ALGEBRAIC APPROACHES TO RESOURCE CONSERVATION VIA PROCESS INTEGRATION

A Dissertation

by

ABDULAZIZ MOHAMMED ALMUTLAQ

Submitted to the Office of Graduate Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

August 2005

Major Subject: Chemical Engineering

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ABSTRACT

Algebraic Approaches to Resource Conservation via Process Integration.

(August 2005)

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The primary objective of this dissertation is to introduce several algebraic procedures to the targeting of material recycle networks. The problem involves the allocation of process streams and fresh sources to process units (sinks) with the objective of minimizing fresh purchase and waste discharge. In the case of composition-limited sinks, allocation to process sinks is governed by feasibility constraints on flowrates and compositions. A systematic non-iterative algebraic approach is developed to identify rigorous targets for minimum usage of fresh resources, maximum recycle of process resources and minimum discharge of waste. These targets are identified a priori and without commitment to the detailed design of the recycle/reuse network. The approach is valid for both pure and impure fresh resources. The devised procedures also identifies the location of the material recycle pinch point and addresses its significance in managing process sources, fresh usage, and waste discharge. The dissertation also addresses the targeting of material-recycle networks when the constraints on the process units are described through flowrates and properties. This property-integration problem is solved using a non-iterative cascade-based algebraic procedure. Finally, for more complex cases with multiple fresh sources and with interception networks, a mathematical-programming approach is developed. Because of the nonlinear non-convex characteristics of the problem, the mathematical model is reformulated to enable the global solution of the problem. Several case studies are solved to illustrate the ease, rigor, and applicability of the developed targeting technique.

DEDICATION

To my dear mother, for all the love, support and guidance throughout the course of my life.

ACKNOWLEDGMENTS

I am grateful to the many people that have guided or helped me throughout the course of my academic career, especially to my remarkable advisor, Dr. Mahmoud M. El-Halwagi.

I greatly appreciate the guidance that my advisor had to offer me, not only in class and research, but also in my personal life. Thank you so much Dr. El-Halwagi.

I am much privileged to work with faculty and graduate students of such top caliber, both at Auburn, my previous school, and at Texas A&M University. Special thanks go to Nimir, Mukund, Vasiliki, Meteab, Abdullah, Musad, Fred, Dustin and Georgina Harell, and Qin.

And lastly, but certainly not the least, much of my gratitude goes to all my family for the support and love through the course of this quest.

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CHAPTER I

INTRODUCTION

1.1 Summary

Resource conservation is becoming the prevailing factor in process industry sustainability nowadays due to market competitiveness and ever evolving stringent environmental regulations, several strategies can lead to that goal among them material recycle/reuse strategy. In this work, an algebraic approach to the targeting of material recycle has been developed. The devised method is non-iterative, systematic and leads to the identification of rigorous targets for minimum usage of fresh resources, maximum recycle of process resources, and minimum discharge of waste. All these targets are determined ahead of detailed design of the recycle/reuse network. These targets are unique and are independent of any assumed mixing arrangements, the devised procedures also identifies the location of the material recycle pinch point. The approach is valid for both pure and impure fresh resources.

1.2 Introduction

Limited supply of natural resources and the chemical industry quest for sustainability coupled with increasingly stringent environmental regulations are enough compelling factors for process industries to pursue more efficient means toward resource conservation.

This dissertation follows the style of *International Journal of Environment and Pollution.*

The tactic of end of pipe treatment is no longer a viable option toward industrial growth. Several strategies such as process modification, material substitution, reaction alteration, and material recycle/reuse can be employed to conserve resources.

Energy crises in late seventies brought up the awareness to look for means to minimize or reduce the consumption and waste of resources, since then numerous techniques have been developed and successfully put into practice.

It is essential to provide a non-iterative, systematic algebraic approach that is able to identify process allocation/modification to further minimize the usage of fresh resources priori of detailed design of the recycle/reuse network. Many insights can be derived and utilized to expand the problem to multiple fresh resource formulation, a more likely industrial scenario, to achieve optimal utilization of resources by process allocation and modification.

1.3 Problem Statement

A typical plant consists of many process streams (sources) and process units (sinks) in order to satisfy a specific task. Minimizing cost for satisfying the demands of the process may include routing of streams, modifications of process variables and purification (interception) of streams. First, the problem is analyzed to allocate sources to sinks only, and then is expanded to the options of process modifications and purification of streams to satisfy the demands of the sinks at minimal cost.

The problem statement is that for a given process there is:

- A set of process sinks (units): $\text{SINKS} = \{j \mid j = 1, \cdots, N_{sinnks}\}$. Each sinks requires a given flowrate, G_j, and a given composition, z_j^{in}, that satisfies the following constraint:

  $$z_j^{\min} \le z_j^{\text{in}} \le z_j^{\max} \qquad \forall j \in \{1, \cdots, N_{sinks}\} \tag{1.1}$$

  where $z_j^{\min}$ and $z_j^{\max}$ are given lower and upper bounds on acceptable compositions to unit j.

- A set of process sources: $\text{SOURCES} = \{i \mid i = 1, \cdots, N_{sources}\}$ which can be recycled/reused in process sinks. Each source has a given flowrate, F_i, and a given composition, y_i^{in}.

- A set of interception units: $\text{INTERCEPTORS} = \{k \mid k = 1, \cdots, N_{\text{int}}\}$ that can be used to remove the targeted species from the sources.

- Available for service is a set of fresh resources: $\text{FRESH} = \{n \mid n = 1, \cdots, N_{fr}\}$ that can be purchased to supplement the use of process sources.

1.4 Objectives

The following objectives for the problem statement are proposed:

1. Algebraic targeting methodology for resource conservation via material recycle/reuse networks through usage of pure fresh resource.
2. Algebraic targeting methodology for resource conservation via material recycle/reuse networks through usage of impure fresh resource.

3. Applicability of the targeting approach to property integration for resource conservation.
4. Cost effective approach toward optimal selection of fresh resources.
5. Advances in the material recycle/reuse network via process interception

The goal of the first objective is to develop a non-iterative algebraic procedure aimed at determining the target for minimum pure fresh resource usage, which ultimately lead to maximizing the usage of process sources, and minimizing waste discharge ahead of detailed design.

The second objective tackle the applicability of the approach developed in the first objective toward targeting for minimum impure fresh resource usage.

The third objective is to test the applicability of the method to the complex structure of property integration for property operators less and greater than process stream operators.

The target for the most economically combination of fresh resources and the demarcation between economical and thermal pinch point is the aim of the fourth objective.

The fifth objective is aimed at developing a concise approach toward interception of process sources in order to minimize the usage of external sources that leads to minimizing the operating cost of the plant as a whole.

1.5 Procedure

The purpose of this work is to introduce a systematic algebraic approach based on El-Halwagi et al. (2003) technique for rigorously targeting minimum usage of fresh resources through material recycle/reuse techniques that overcomes the graphical technique limitations. The proposed approach can be automated using spreadsheets and can be integrated with other computations techniques for process design and optimization to identify the target for minimum usage of fresh resources ahead of detailed design without commitment to the final network configurations and to retrofit existing network through process modification. The broad applicability and ease of implementation of this new method will be shown and verified by solving several case studies published in literature. An outline of the procedure is as follows:

Application of the proposed algebraic targeting approach to property integration is to be examined, especially for the case where fresh property operator is greater than the process stream operator.

The procedure to accomplish the fourth objectives in the problem statement is to algebraically identify optimal conditions for selecting fresh resources that can be employed for the process.

Finally, the last objective of this proposal is to develop a global optimization formulation for process modification and interception to satisfy a typical plant demand.

CHAPTER II

ALGEBRAIC TARGETING FOR PURE FRESH RESOURCES

2.1 Literature Review

Depletion of natural resources is a common characteristic of the chemical process industries. Consequently, the process industries have been under increasing pressure to develop resource conservation strategies that are aimed at reducing the consumption of fresh resources and mitigating the discharge of pollutants. A particularly effective strategy for resource conservation and waste reduction is recycle/reuse.

Recent research efforts have been geared towards developing systematic procedures to minimize the usage of fresh resources using network synthesis and analysis. The problem of synthesizing mass exchange networks (MENs) was introduced by El-Halwagi and Manousiouthakis (1989) who developed a targeting technique to identify maximum extent of mass exchange among process streams and minimum usage of external lean streams. An important variation of MENs, wastewater minimization, was introduced by Wang and Smith (1994) who developed a graphical targeting approach to minimize fresh water consumption and wastewater discharged by the transfer of contaminants from process streams to water streams. In this approach, the basic process unit is modeled as a mass exchanger.

Dhole et al. (1996) and El-Halwagi and Spriggs (1996) addressed the problem of water usage and discharge through a source (supply)-sink (demand) representation. The sinks are not limited to being mass-exchange units. This problem will be referred to as the ***recycle/reuse problem*** and is the focus of these investigations. The objective of the recycle/reuse problem is to allocate various process sources (or streams) to sinks (units that can employ the sources) so as to minimize the consumption of the fresh resource (e.g., fresh water). Dhole et al. (1996) developed a graphical representation of concentration versus flowrate. Sources and sinks are independently compiled in supply and demand composite curves that are integrated until a pinch point is created. El-Halwagi and Spriggs (1996) developed a source-sink mapping diagram along with lever-arm rules that identify optimal allocation of sources to sinks. Polley and Polley (2000) determined optimality conditions for sequencing recycles. Additionally, Sorin and Bedard (1999) developed an iterative algebraic method called the evolutionary table, it is based on mixing source streams at concentrations bordering the demand location and moving on progressively to higher concentration. The procedure also sets guidelines for maximizing the reuse of process water. The method may become cumbersome for systems with large number of sources and sinks. Hallale (2002) introduced a technique that identifies global pinch points that may be missed by the evolutionary table by coupling the water surplus diagram with a graphical representation of purity versus flowrate. The idea of surplus was also developed by Alves (1999) and Alves and Towler (2002) for the application of hydrogen recovery systems in refineries. This approach requires extensive calculations and there is a dependence of two graphs to satisfy flowrate and composition for the source-sink structure. Manan et al. (2004) refined the surplus approach to avoid the extensive calculations in identifying the targets. El-Halwagi et al. (2003) developed a graphical technique (material recycle pinch analysis) to identify targets for minimum usage of fresher source, maximum integration of process recycles, and minimum discharge of waste.

Mathematical programming techniques have also been used to solve the recycle/reuse problems using optimization techniques (e.g., Takama et al. (1980), Alva-Argáez et al. (1998, 1999), Keckler and Allen (1999), Benko et al. (2000) and Dunn et al. (2001), Savelski and Bagajewicz. (2000, 2001).

The objective of this study is to introduce an algebraic technique for the recycle/reuse problems. The technique provides a computational analogue to the graphical approach developed by El-Halwagi et al. (2003) and sets the basis for minimizing fresh resource usage by implementing segregation, mixing, and direct recycle/reuse strategies. A cascade representation is used to track flows and loads throughout the system. Next, optimality conditions are embedded in the cascade calculations. The devised approach identifies rigorous targets for minimum usage of fresh resources, maximum recycle of process sources to process units, and minimum discharge of waste. Several case studies from literature are solved to illustrate the applicability and merits of the developed algebraic procedure.

2.2 Problem Statement

Consider a process with:

- A number ($N_{sources}$) of process streams (or sources) that are considered for recycle/reuse. Each source, i, has a flowrate W_i, and composition y_i, $i = 1,2,\ldots,N_{sources}$.
- A number (N_{sinks}) of process units (sinks). Each sink, j, can accommodate a feed of given flowrate G_j, with z_j^{in} composition that lies within predefined upper and lower bounds $z_j^{\min}$ *and* $z_j^{\max}$, j=1, 2,…, N_{sinks} .

- Pure fresh (external) resource that can be purchased to supplement the use of process sources in sinks.

The objective is to develop a non-iterative algebraic procedure aimed at minimizing the purchase of fresh resource, maximizing the usage of process sources, and minimizing waste discharge.

2.3 Problem Formulation Background

The problem formulation and optimality conditions via dynamic programming were derived by El-Halwagi et al. (2003). A brief description of their work is given below. The process as well as fresh sources are first split into fractions (equal in number to the sinks plus an extra one to accommodate the unused portion of any process stream) of unknown flowrate. Material balance is done around the splitters and mixers, then the objective is to minimize the amount of fresh resources by maximizing the utilization of the process sources. Dynamic programming was utilized to derive the mathematical conditions of an optimal solution policy. In particular, two optimality rules were derived:

- **Sink Composition Rule:** When a fresh resource is mixed with process source(s), the composition of the mixture entering the sink should be set to a value that minimizes the fresh arm. For instance, when the fresh resource is a pure substance that can be mixed with pollutant-laden process sources, the composition of the mixture should be set to the maximum admissible value.
- **Source Prioritization Rule:** In order to minimize the usage of the fresh resource, recycle of the process sources should be prioritized in order of their fresh arms starting with the source having the shortest fresh arm.

El-Halwagi et al. (2003) transformed these optimality rules in a graphical targeting procedure referred to as "Material Recycle Pinch Diagram) and can be summarized as follows:

1. Rank the sinks in ascending order of maximum admissible composition, $z_1^{\max} \le z_2^{\max} \le \ldots z_j^{\max} \ldots \le z_{N_{Sinks}}^{\max}$
2. Rank sources in ascending order of pollutant composition, i.e. $y_1 < y_2 < \ldots y_i \ldots\ldots < y_{N_{Sources}}$
3. Calculate the maximum load of each sink as follows:

$$M_j^{Sink,\max} = G_j z_j^{\max} \tag{2.1}$$

4. Plot the maximum load of each sink versus its flowrate. Create a sink composite curve by superposition of the sinks arrows in ascending order.
5. Calculate the source load as follows:

$$M_i^{Source} = W_i y_i \tag{2.2}$$

6. Plot the load of each source versus its flowrate. Create a source composite curve by superposition of the sources in ascending order.
7. Move the source composite stream till it touches the sink composite stream with the source composite below the sink composite in the overlapped region. The point where they touch is the material recycle/reuse pinch point. The flowrate of sinks below which there are no sources is the target for minimum fresh discharge. On the other hand, the flowrate of the sources above which there are no sinks is the target for waste discharge.

The results of this targeting procedure are presented in Figure 2.1. They illustrate the minimum usage of fresh materials, maximum extend of direct recycle, and minimum discharge of waste.

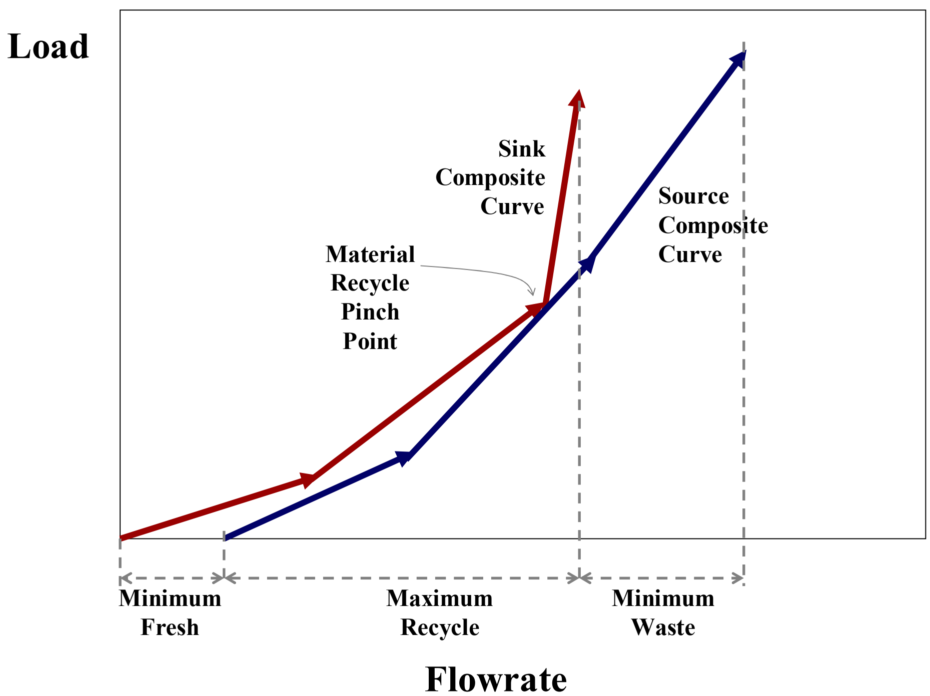


Figure 2.1 Material recycle pinch diagram (El-Halwagi et al. 2003).

In spite of the usefulness of this graphical targeting procedure in locating material recycle/reuse pinch point, minimum fresh resource, maximum recycle, and minimum waste discharge of material, it has two key limitations:

1. Scale Problems: When there is a large range of loads or flows involved in the problem, the accuracy of the graph may diminish.
2. Size Problems: When there are numerous sources and sinks, it may be cumbersome to plot all the streams and units in the process.

In this work, an algebraic procedure that overcomes these limitations has been developed. The procedure can also be automated using spreadsheets and can be integrated with other computations techniques for process design and optimization to identify the target for minimum usage of fresh resources ahead of detailed design without commitment to the final network configurations and to retrofit existing network through debottlenecking and process modification.

2.4 Algebraic Targeting Procedure

In order to develop the algebraic targeting procedure, let us revisit Figure 2.1 and adjust it by sliding the source composite curve all the way to the left (to start from the origin) as shown in Figure 2.2. In so doing, we create infeasibility that can be described in a couple of ways by looking vertically and horizontally. At a given flowrate, the source composite lies above the sink composite, thereby violating the maximum load admissible to the sink. An alternative way of describing the infeasibility is that for a given load, the source composite lies to the left of the sink composite, thereby leading to a shortage of the flowrate necessary for the sink. The maximum infeasibility corresponds to the maximum shortage of flowrate which is designated as $\delta_{\max}$. Indeed, all infeasibilities are eliminated by sliding the source composite curve to the right a distance equal to $\delta_{\max}$ (Figure 2.3). Consequently, the target for minimum fresh usage is equal to the maximum shortage, i.e.

$$\text{Target for Minimum Fresh Consumption } = \delta_{\max} \tag{2.3}$$

Our objective is to evaluate this maximum shortage algebraically without the need to resort to the graphical representation.

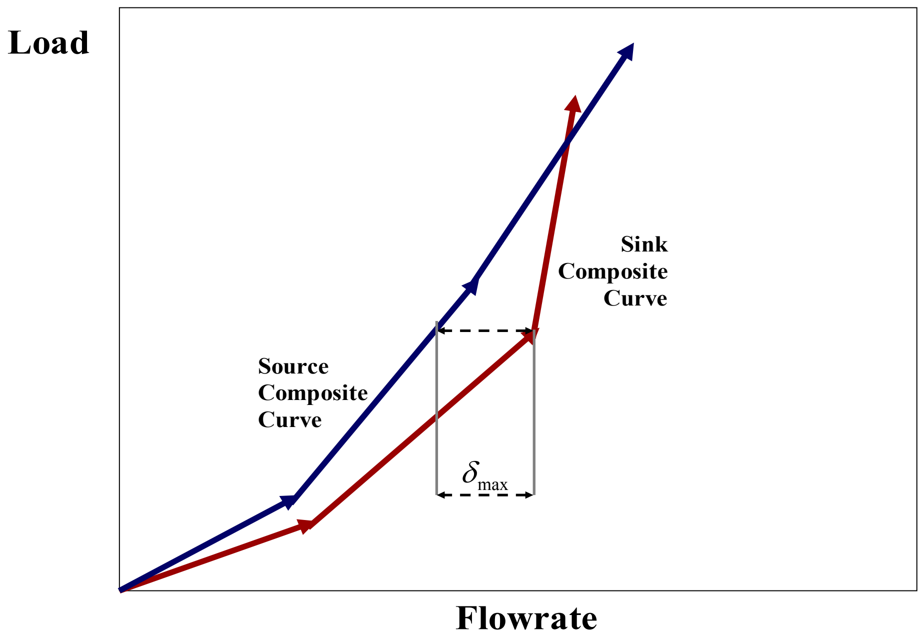


Figure 2.2 Sliding the source composite to left generate infeasibility.

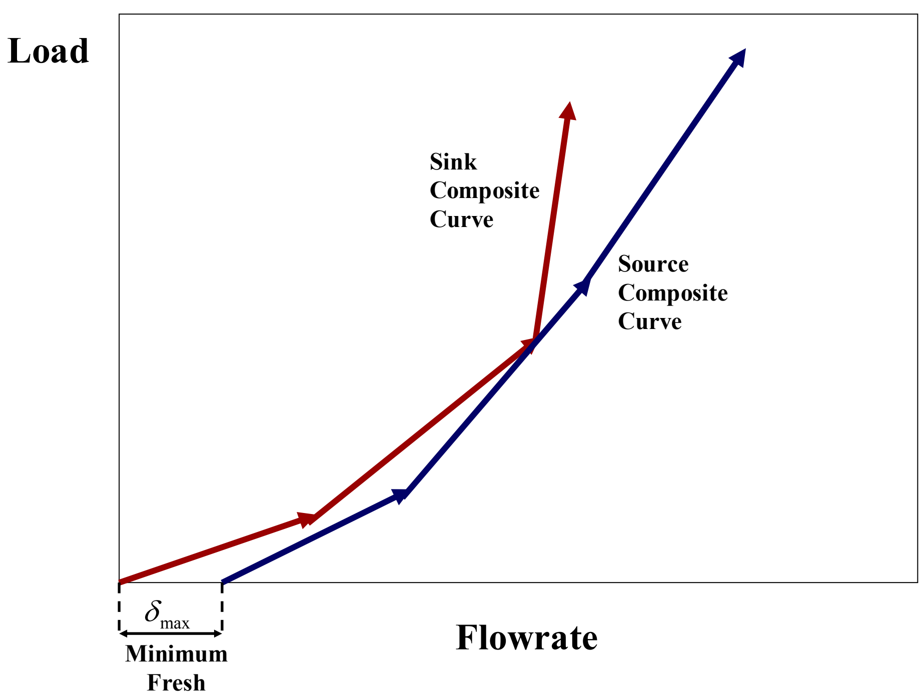


Figure 2.3 Minimum fresh target correspond to maximum flow shortage.

Let us revisit Figure 2.2 and draw horizontal lines at corner points (kinks) of the source- and sink-composite curves (Figure 2.4). These horizontal lines are numbered through index k which starts with k = 0 at the zero load level and go up at each horizontal level. The load at each horizontal level, k, is referred to as M_k. The vertical distance between each two horizontal lines is referred to as a *load interval* and is given the index k as well. The load within interval k is calculated as follows:

$$\Delta M_k = M_k - M_{k-1} \tag{2.4}$$

Next, we calculate the flowrates of the source and the sink within interval k. These correspond to the horizontal distances on the source- and sink-composite curves contained within the interval. Hence, they can be calculated as:

$$\Delta W_k = \frac{\Delta M_k}{y_{\text{source in interval k}}} \tag{2.5}$$

and

$$\Delta G_k = \frac{\Delta M_k}{z^{\max}_{\text{sink in interval k}}} \tag{2.6}$$

Figure 2.4 illustrates the concepts of a load interval and flowrates of sources and sinks within an interval. Another important observation from Figure 2.4 is that at any horizontal level ($\bar{k}$), the horizontal distance between the source- and the sink-composite curves is given by:

$$\delta_{\bar{k}} = \sum_{k=1}^{\bar{k}} W_k - \sum_{k=1}^{\bar{k}} G_k \tag{2.7}$$

This expression can be verified from Figure 2.4 and is consistent with the observation that at any load, the horizontal distance between the source- and the sink-composite curves is the difference in cumulative flowrates. A negative value of δ indicates infeasibility (the source composite lies to the left of the sink composite). Applying Equation (2.7) to the first interval, we get:

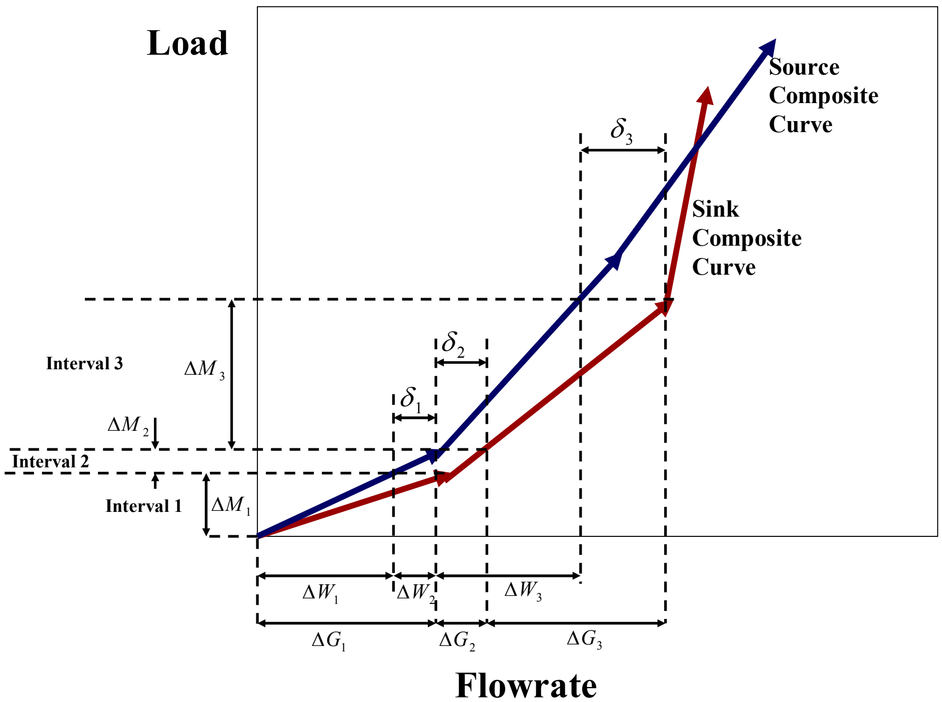


Figure 2.4 Load intervals, flows, and residuals.

$$\delta_1 = \Delta W_1 - \Delta G_1 \tag{2.8}$$

This result can be verified by Figure 2.4. Similarly, applying Equation (2.7) to the second interval, we have:

$$\delta_2 = \Delta W_1 + \Delta W_2 - \Delta G_1 - \Delta G_2 \tag{2.9}$$

Substituting from Equation (2.8) into Equation (2.9), we obtain

$$\delta_2 = \delta_1 + \Delta W_2 - \Delta G_2 \tag{2.10}$$

and, for the k^{th} interval:

$$\delta_k = \delta_{k-1} + \Delta W_k - \Delta G_k \tag{2.11}$$

with $\delta_0 = 0$. Equation (2.11) is represented by Figure 2.5. The flow balances can be carried out for all intervals resulting in the cascade diagram shown on Figure 2.6. On the cascade diagram, the most negative value of δ (referred to as $\delta_{\max}$) corresponds to the target for minimum fresh consumption as indicated by Equation (2.3). Additionally, in order to remove the infeasibilities a flowrate of the fresh resource equal to $\delta_{\max}$ is added to the top of the cascade (i.e., $\delta_0 = \delta_{\max}$) and the residuals from all intervals are adjusted. The result is that the most negative residual now becomes zero indicating the pinch location. Furthermore, the revised residual leaving the last interval is the target for minimum wastewater discharge. These results are shown on the revised cascade diagram illustrated by Figure 2.7.

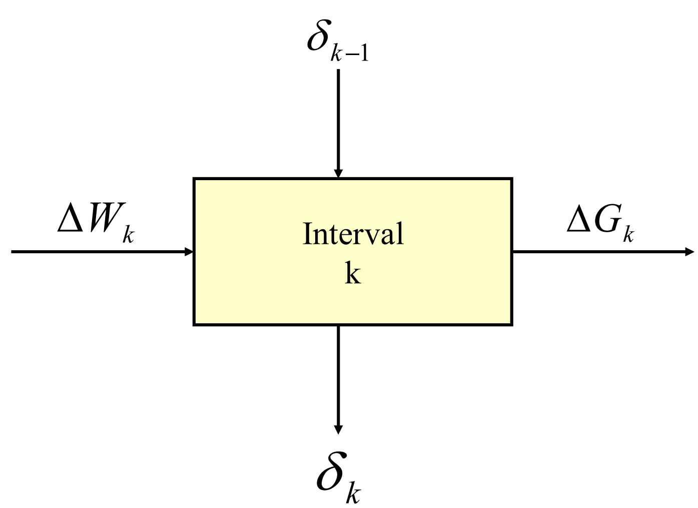


Figure 2.5 Flow balance around a load interval for pure fresh resources.

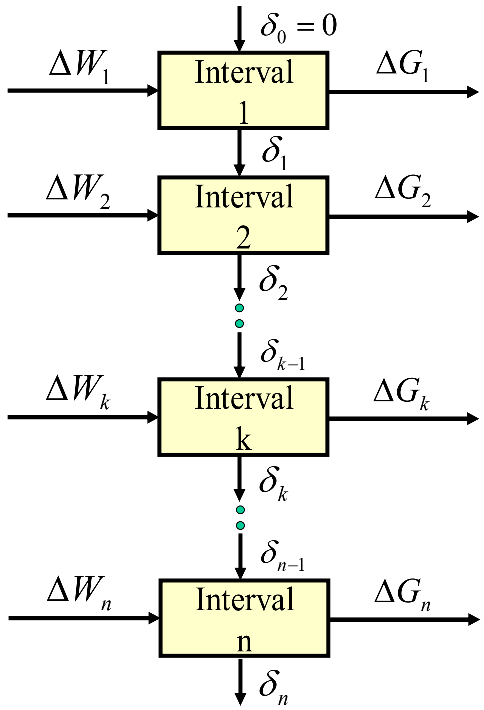


Figure 2.6 Cascade diagram for pure fresh resources.

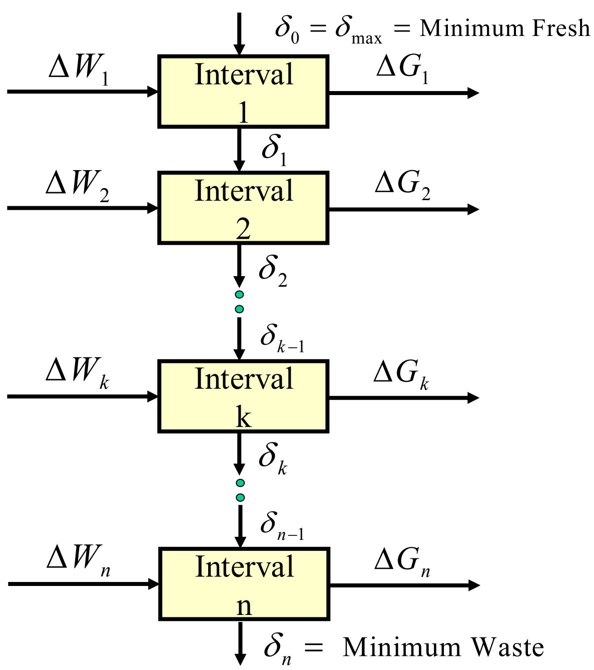


Figure 2.7 Revised cascade diagram for pure fresh resources.

Based on the foregoing analysis, the algebraic procedure can be summarized as follows:

1. Rank the sinks in ascending order of maximum admissible composition, $z_1^{\max} \leq z_2^{\max} \leq \ldots z_j^{\max} \ldots \leq z_{N_{Sinks}}^{\max}$
2. Rank sources in ascending order of pollutant composition, i.e. $y_1 < y_2 < \ldots y_i \ldots.. < y_{N_{Sources}}$
3. Calculate the load of each sink ($M_j^{Sink,\max} = G_j z_j^{\max}$) and source ($M_i^{Source} = W_i y_i$).
4. Compute the cumulative loads for the sinks and for the sources (by summing up their individual loads).
5. Rank the cumulative loads in ascending order.
6. Develop the load-interval diagram (LID) shown in Figure 2.8. First, the loads are represented in ascending order starting with zero load. The scale is irrelevant. Next, each source (and each sink) is represented as an arrow whose tail corresponds to its starting load and head corresponds to it ending load. Equations (2.4)-(2.6) are used to calculate the intervals load, source flowrate, and sink flowrate.
7. Based on the interval source- and sink flowrates, develop the cascade diagram and carry out flow balances around the intervals to calculate the values of the flow residuals (δ_k's). The most negative δ_k is the target for minimum fresh consumption.
8. Revise the cascade diagram by adding the maximum δ_k to the first interval and calculate the revised residuals. The residual flow leaving the last interval is the

target for minimum waste discharge. The interval with the first zero residual is the material recycle/reuse global pinch point.

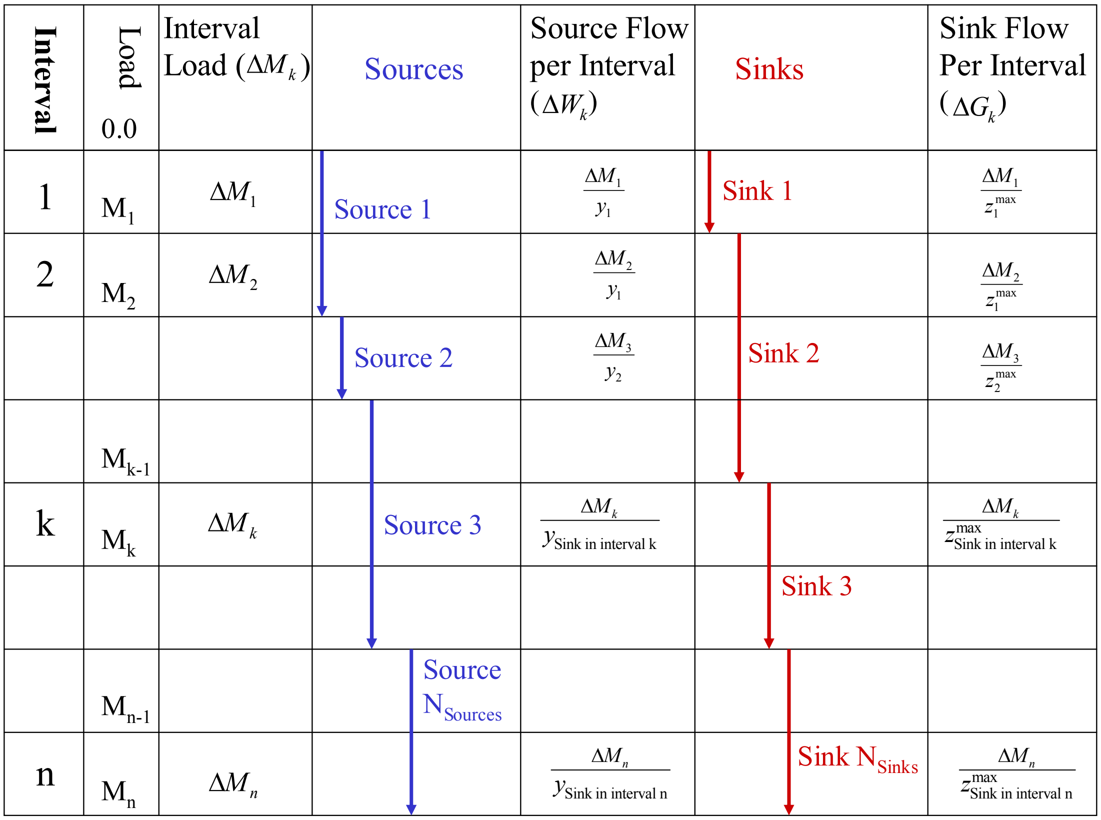


Figure 2.8 Load interval diagram for pure fresh resources.

2.5 Case Studies

In the following examples, we illustrate the applicability of the developed procedure using two case studies:

Example 1. This case study is taken from Polley and Polley (2000). The study has four sources and four sinks and information concerning them can be seen below in Table 2.1 and Table 2.2. The LID is illustrated in Figure 2.9. The cascade diagram is given by Figure 2.10(a). As can be seen, the most negative residual is –70 tons/hr. Therefore, the target for minimum fresh water is 70 ton/hr. When this value is added to the first interval, we can carry out the revised cascade calculations leading to a target of minimum wastewater discharge (residual leaving last interval) of 50 tons/hr. The zero residual designates the pinch location. Hence, the material recycle pinch point is located at the horizontal lines separating intervals 5 and 6. As can be seen from the LID, this location corresponds to a cumulative load of 14 kg/hr and a contaminant concentration of 150 ppm (between intervals 5 and 6 which corresponds to 150 ppm on the source side).

Table 2.1 Source information for Polley and Polley case study (Polley and Polley 2000).

Sources	**Flow, ton/hr**	**Concentration, ppm**	**Load, kg/hr**	**Cumulative Load, kg/hr**
1	50	50	2.5	2.5
2	100	100	10	12.5
3	70	150	10.5	23.0
4	60	250	15	38.0

Table 2.2 Sink information for Polley and Polley case study (Polley and Polley 2000).

Sinks	**Flow, ton/hr**	**Maximum Inlet Concentration, ppm**	**Maximum Inlet Load kg/hr**	**Cumulative Load, kg/hr**
1	50	20	1	1.0
2	100	50	5	6.0
3	80	100	8	14.0
4	70	200	14	28.0

Interval	Load, kg/hr 0.0	Interval Load (ΔM_k) kg/hr	Sources	Source Flow per Interval (ΔW_k), ton/hr	Sinks	Sink Flow Per Interval (ΔG_k), ton/hr
1	1.0	1.0	Source 1 y = 50	20	Sink 1 z^{max}=20	50
2	2.5	1.5		30	Sink 2 z^{max}=50	30
3	6.0	3.5	Source 2 y = 100	35		70
4	12.5	6.5		65	Sink 3 z^{max}=100	65
5	14.0	1.5	Source 3 y = 150	10		15
6	23.0	9.0		60	Sink 4 z^{max}=200	45
7	28.0	5.0	Source 4 y = 250	20		25
8	38.0	10.0		40		0

Figure 2.9 LID for Polley and Polley case study.

Example 2. To illustrate the effectiveness of the method in identifying the global pinch point, Sorin and Bedard (1999) case study is explored next. Six processes containing a single contaminant, each process has an inlet and outlet water flowrate and contaminant concentration with the exception of Process 3 where the entire flowrate is depleted internally. The data for the processes is presented in Table 2.3 and Table 2.4.

The first step in the targeting procedure is to identify the sinks and sources and ranked them in terms of ascending concentration levels. The individual load for each stream in the process is calculated and cumulative loads for the sinks and sources are obtained. The cumulative load for the whole process is then arranged in ascending order to obtain the number of intervals followed by calculating the flowrates of the sinks and sources through each interval as shown in Figure 2.11. Since the contaminant concentration is zero for the first interval sink, its flowrate can be determined using L'Hopital's rule as shown below:

$$\Delta G_1 = \frac{\Delta M_1}{z_{1 \text{ in interval } 1}^{\max}} = \frac{d(\Delta M_1)}{d(z_{1 \text{ in interval } 1}^{\max})} = G_1 \tag{2.12}$$

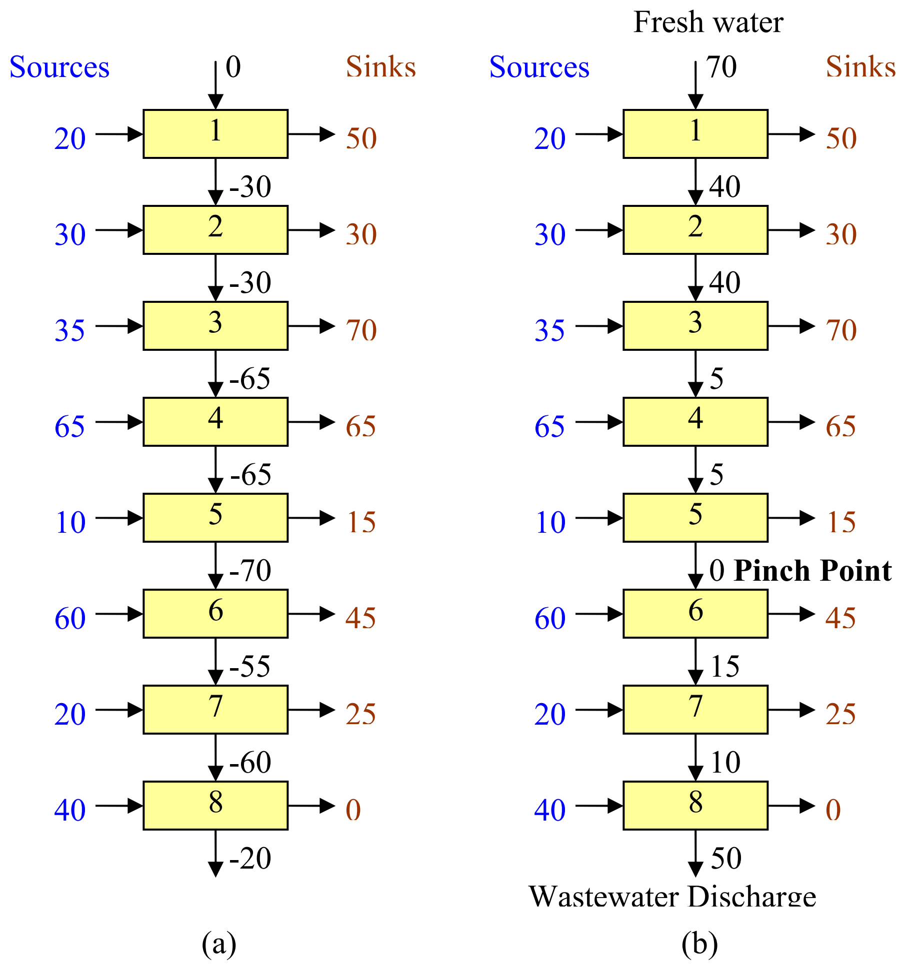


Figure 2.10 Cascade diagram for Polley and Polley case study, (a) with infeasibilities (b) revised.

Table 2.3 Source information for Sorin and Bedard case study (Sorin and Bedard 1999).

Sources	**Flow, ton/hr**	**Concentration, ppm**	**Load, kg/hr**	**Cumulative Load, kg/hr**
1	120	100	12.0	12.0
2	80	140	11.2	23.2
3	140	180	25.2	48.4
4	80	230	18.4	66.8
5	195	250	48.75	115.55

Table 2.4 Sink information for Sorin and Bedard case study (Sorin and Bedard 1999).

Sink	**Flow, ton/hr**	**Maximum Inlet Concentration, ppm**	**Maximum Inlet Load kg/hr**	**Cumulative Load, kg/hr**
1	120	0	0.0	0.0
2	80	50	4.0	4.0
3	80	50	4.0	8.0
4	140	140	19.6	27.6
5	80	170	13.6	41.2
6	195	240	46.8	88.0

Interval	Load kg/hr 0.0	Interval Load (ΔM_k) kg/hr	Sources	Source Flow per Interval (ΔW_k), ton/hr	Sinks	Sink Flow per Interval (ΔG_k), ton/hr
1	0	0		0.00	Sink 1 $z^{maz}=0$	120.00
2	4	4		40.00	Sink 2 $z^{maz}=50$	80.00
3	8	4	Source 1 y =100	40.00	Sink 3 $z^{maz}=50$	80.00
4	12	4		40.00		28.57
5	23.2	11.2	Source 2 y =140	80.00	Sink 4 $z^{maz}=140$	80.00
6	27.6	4.4		24.44		31.43
7	41.2	13.6	Source 3 y =180	75.56	Sink 5 $z^{maz}=170$	80.00
8	48.4	7.2		40.00		30.00
9	66.8	18.4	Source 4 y =230	80.00	Sink 6 $z^{maz}=240$	76.67
10	88.0	21.2	Source 5 y =250	84.80		88.33
11	115.55	27.55		110.20		0.00

Figure 2.11 LID for Sorin and Bedard case study.

The cascade diagram is then constructed starting with no fresh water. The most negative residual value indicates the minimum amount of fresh water must be supplied to the process in order to accomplish the required task, as can be seen from Figure 2.12 the minimum freshwater is 200 ton/hr and the minimum wastewater discharge is 120 ton/hr. These values agree exactly with those found by Sorin and Bedard (2000) using their algebraic Evolutionary Table method. Additionally, the graph identifies two pinch points at 100 and 180 ppm conforming to Hallale's (2002) findings.

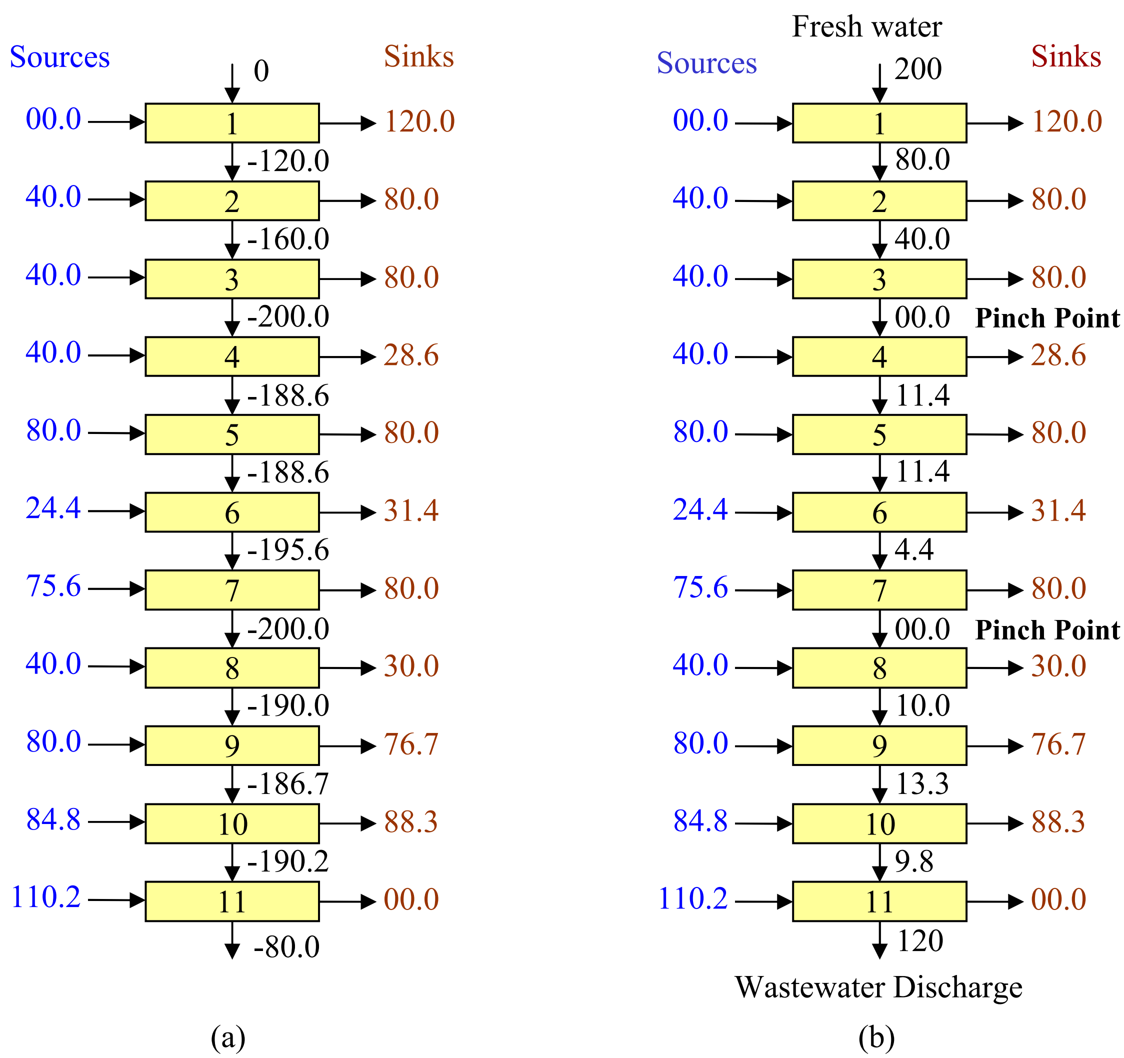


Figure 2.12 Cascade diagram for Sorin and Bedard case study, (a) with infeasibilities (b) revised.

2.6 Conclusions

This paper has introduced an algebraic method for the rigorous targeting of material recycle/reuse networks. Sink and source optimality rules have been used to construct a load-interval diagram that constitutes the basis for a non-iterative cascade calculations. The developed cascade procedure systematically identifies minimum usage of fresh resource, maximum recycle/reuse of process resources, and minimum discharge of waste. Additionally, the procedure identifies the location of material recycle/reuse pinch points. Two case studies have been used to illustrate the applicability of the devised procedure.

Application of the method to impure fresh resources as well as investigating the presence of multiple fresh resources is recommended for future studies.

2.7 Nomenclature

G Sink (unit) flow, mass or volume/time

M Load, mass or volume/time

$N_{sources}$ Number of process streams (or sources)

N_{sinks} Number of process units (sinks)

W Sink (unit) flow, mass or volume/time

y Contaminant composition of process streams (or sources)

z Allowable contaminant composition of process unit (or sink)

$\bar{k}$ Total number of intervals

Superscripts

min Unit (sink) lower bound of allowable contaminant concentration

max Unit (sink) upper bound of allowable contaminant concentration

Subscripts

i Index for sources

j Index for sinks

k Interval index

Greek Letters

δ Interval Residual, mass or volume/time

Δ Difference between two consecutive intervals

CHAPTER III

ALGEBRAIC TARGETING FOR IMPURE FRESH RESOURCES

3.1 Literature Review

The process industries have a critical role to play in ensuring environmental sustainability and judicious development. Sustainable development is defined as "the development which meets the needs of the present without compromising the ability of future generations to meet their own needs" (Bruntland Report, 1987). Because of the tremendous consumption of natural resources by the process industries, it is necessary to develop material conservation and waste reduction strategies that are conducive to sustainable development while providing cost-effective solutions to industry. In this context, recycle/reuse is recognized as one of the most desirable and cost-effective approaches for material conservation and waste reduction.

A number of researchers have addressed the issues involved in designing recycle/reuse systems. Takama et al. (1980) proposed the use of mathematical programming techniques to solve water recycle problems. Several researchers adopted and generalized this approach (e.g., Alva-Argaez et al., 1999; Keckler and Allen, 1999; Benko et al., 2000; Savelski and Bagajewicz, 2000, 2001; and Dunn et al., 2001). Additionally, systematic methods have been developed for unsteady-state and batch recycle systems (e.g., Wang and Smith, 1995; Almato et. al., 1997; and Puigjaner, 1999).

Several visualization techniques have also been developed to address wastewater minimization problems. Wang and Smith (1994) developed a graphical targeting approach to minimize fresh water consumption and wastewater discharged while transferring contaminants from process streams to water streams in units that function as mass exchangers. Dhole et al. (1996) and El-Halwagi and Spriggs (1996) observed that not all units can be modeled as mass exchangers. They treated the problem of material usage and discharge through a source (supply)-sink (demand) representation. This problem will be referred to as the recycle/reuse problem in which various process sources (or streams) are allocated to sinks (units that can employ the sources) so as to minimize the consumption of the fresh resource (e.g., fresh water). Dhole et al. (1996) developed a graphical representation of concentration versus flowrate; sources and sinks are independently compiled in supply and demand composite curves that are integrated until a pinch point is created. El-Halwagi and Spriggs (1996) employed the lever-arm rules on a source-sink mapping diagram that identify optimum allocation of sources to sinks. Polley and Polley (2000) outlined optimality conditions for sequencing recycles. The evolutionary table was introduced by Sorin and Bedard (1999) in an attempt to solve the recycle/reuse problem algebraically. It is based on mixing source streams at concentrations bordering the demand location and moving on progressively to higher concentration. The procedure also sets guidelines for maximizing the reuse of process water. The method may become cumbersome for systems with large number of sources and sinks. Hallale (2002) introduced a technique that identifies global pinch points that may be missed by the evolutionary table by coupling the water surplus diagram with a graphical representation of purity versus flowrate. The idea of surplus was also developed by Alves (1999) and Alves and Towler (2002) for the application of hydrogen recovery systems in refineries. This approach requires extensive calculations and there is a dependence of two graphs to satisfy flowrate and composition for the source-sink structure. Manan et al. (2004) refined the surplus approach to avoid the extensive calculations in identifying the targets.

El-Halwagi et al. (2003) developed a graphical technique for material recycle referred to as the material recycle pinch analysis. This technique was the first visualization approach which solves the source-sink allocation problem non-iteratively. The approach identifies material recycle pinch points along with their optimality criteria. It also determines the targets of minimum usage of fresh sources, maximum integration of process recycles, and minimum discharge of waste. While this graphical technique provides key visualization insights, it is beneficial to develop an algebraic procedure which is particularly useful in the following cases:

- Numerous sources and sinks: As the number of sources and sinks increase, it becomes more convenient to use spreadsheets or algebraic calculations to handle the targeting.
- Scaling problems: If there is a significant difference in values of flowrates and/or loads for some of the sources and/or sinks, the graphical representation becomes inaccurate since the larger flows/loads will skew the scale for the other streams.
- If the targeting is tied with a broader design task that is handled through algebraic computations, it is desirable to use consistent algebraic tools for all the tasks.

The objective of this paper is to introduce an algebraic technique for the recycle/reuse problems. The technique provides a computational analogue to the graphical approach developed by El-Halwagi et al (2003) and sets the basis for minimizing fresh resource usage by implementing segregation, mixing, and direct recycle/reuse strategies. A cascade representation is used to track flows and loads throughout the system. Next, optimality conditions are embedded in the cascade calculations. The devised approach identifies rigorous targets for minimum usage of fresh resources, maximum recycle of process sources to process units, and minimum discharge of waste. Two case studies from literature are solved to illustrate the applicability and merits of the developed algebraic procedure.

3.2 Problem Statement

Consider a process with:

- A number ($N_{sources}$) of process streams (sources) that are candidates for recycle/reuse. Each source, i, has a flowrate W_i, and composition $y_i, i = 1,2,\ldots,N_{sources}$.
- A number (N_{sinks}) of process units (sinks), each sink j can accommodate a feed of given flowrate G_j, with composition, z_j^{in} that lies within predefined upper and lower bounds, $z_j^{\min}$ and $z_j^{\max}$, $j = 1,2,\ldots,N_{sinks}$.
- A fresh (external) resource with a contaminant concentration of y_f that can be purchased to supplement the use of process sources in sinks.

The objective is to develop a non-iterative algebraic procedure aimed at minimizing the purchase of fresh resource, maximizing the usage of process sources, and minimizing waste discharge.

3.3 Problem Formulation Background

The problem formulation and optimality conditions via dynamic programming were derived by El-Halwagi et al. (2003). According to their methodology, the process as well as fresh source is first split into fractions of unknown flowrate and routed to each sink (unit), whereas the unused portion of process sources is directed toward a waste station. Material balances are carried out for the splitters and mixers. The objective is to minimize the amount of fresh resource through maximizing the utilization of the process sources. The mathematical conditions of an optimal solution policy are then driven via dynamic programming; in particular, two optimality rules were derived:

- **Sink Composition Rule**: The composition of the mixture entering the sink should be set to a value that minimizes the fresh arm. For instance, when the fresh resource is a pure substance that can be mixed with pollutant-laden process sources, the composition of the mixture should be set to the maximum admissible value.
- **Source Prioritization Rule**: Recycle of the process sources should be prioritized in order of their fresh arms starting with the source having the shortest fresh arm.

El-Halwagi et al. (2003) transformed these optimality rules into a graphical targeting procedure referred to as "Material Recycle Pinch Diagram" and can be summarized as follows:

1. Rank the sinks in ascending order of maximum admissible composition, $z_1^{\max} \le z_2^{\max} \le \ldots z_j^{\max} \ldots \le z_{N_{Sinks}}^{\max}$
2. Rank sources in ascending order of pollutant composition, i.e. $y_1 < y_2 < \ldots y_i \ldots\ldots < y_{N_{Sources}}$

3. Calculate the maximum load of each sink as follows:

$$M_j^{Sink,\max} = G_j z_j^{\max} \tag{3.1}$$

4. Plot the maximum load of each sink versus its flowrate. Create a sink composite curve by superposition of the sinks arrows in ascending order.
5. Calculate the source load as follows:

$$M_i^{Source} = W_i y_i \tag{3.2}$$

6. Plot the load of each source versus its flowrate. Create a source composite curve by superposition of the sources in ascending order.
7. Move the source composite stream till it touches the sink composite stream with the source composite below the sink composite in the overlapped region. The point where they touch is the material recycle/reuse pinch point. The flowrate of sinks below which there are no sources is the target for minimum fresh discharge. On the other hand, the flowrate of the sources above which there are no sinks is the target for waste discharge.

   The results of this targeting procedure are shown in Figure 3.1.

When impure fresh sources are used, the procedure should be revised to account for the load of impurities introduced by the use of the fresh stream(s). In such cases, the process composite curve is slid over the locus of the fresh source (a line having a slope of the composition of the impurity) until it touches the sinks composite curve as shown in Figure 3.2.

We are now in a position to develop the algebraic procedure based on the aforementioned concepts.

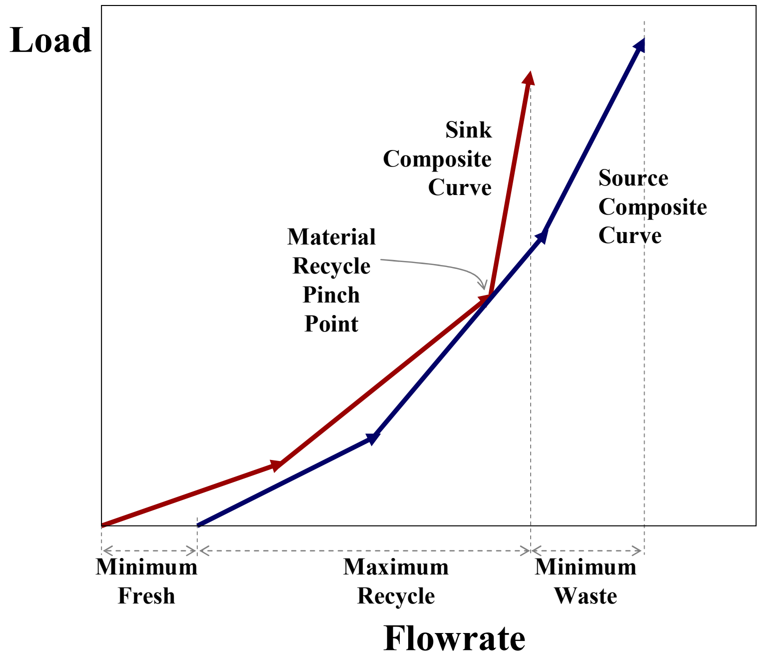


Figure 3.1 Material recycle/reuse for pure fresh resources (El-Halwagi et al., 2003)

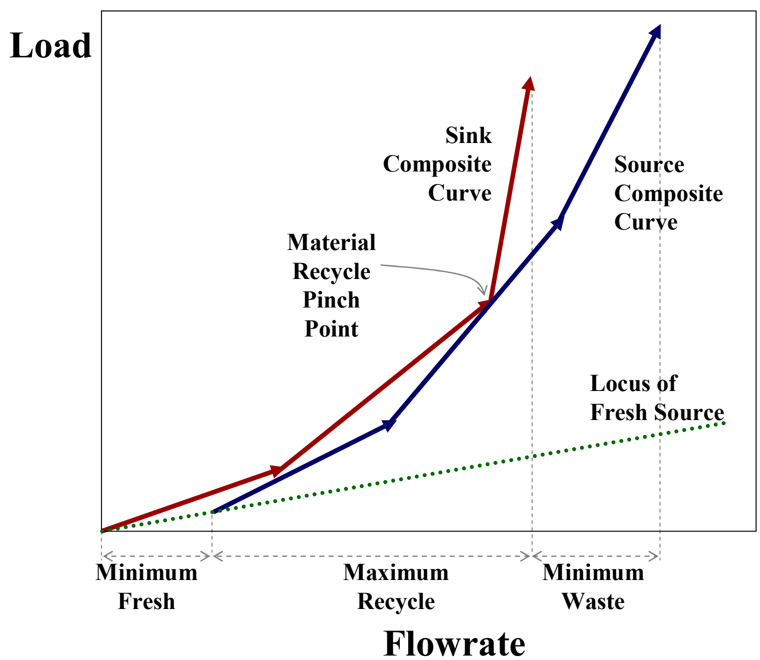


Figure 3.2 Material recycle/reuse pinch diagram for impure fresh resources.

3.4 Derivation of Algebraic Conditions for Feasibility

First, let us start with the case of using a pure fresh source (Figure 3.1). Feasibility conditions dictate that at any given load, the flowrate of sources must be greater than or equal to that of sinks. Figure 3.3 is a re-plot of Figure 3.1 with both composites starting from the origin. Since each composite represents a piecewise linear function, the maximum infeasibility, if transpire, will be at the corner (kink) points. Therefore, let us draw horizontal lines at the corner points (kinks) of the source and sink composites as shown in Figure 3.3. These horizontal lines are numbered using an index k which starts with $k = 0$ at the zero load level and are numbered in ascending order. The load at each horizontal level, k, is referred to as M_k. The vertical distance between each two horizontal lines is referred to as *load interval* and is given the index k as well. The load within interval k is calculated as follows:

$$\Delta M_k = M_k - M_{k-1} \tag{3.3}$$

The flowrates of the source and the sink within interval k correspond to the horizontal distances on the source-sink-composite curves enclosed within the interval. Hence, they can be calculated as follows:

$$\Delta W_k = \frac{\Delta M_k}{y_{\text{source in interval } k}} \tag{3.4}$$

and

$$\Delta G_k = \frac{\Delta M_k}{z^{\max}_{\text{sink in interval } k}} \tag{3.5}$$

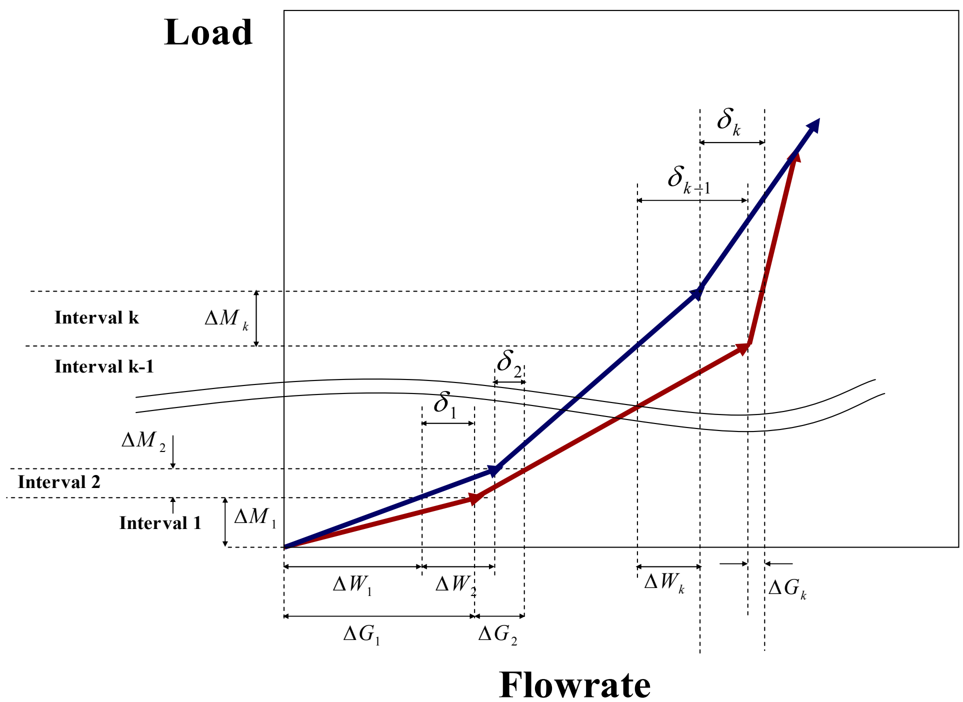


Figure 3.3 Load intervals, flows, and residuals for pure fresh resources.

Let us examine the diagram at several intervals, and set the feasibility conditions for those intervals:

For the first interval, the load is M_1 and the load interval is ΔM_1. Thus:

$$F_1^{Sources} = \frac{\Delta M_1}{y_{\text{source in interval 1}}} = \Delta W_1 \tag{3.6}$$

where $F_1^{Sources}$ is the flowrate of the sources available for use to the sinks in interval 1

$$F_1^{Sink} = \frac{\Delta M_1}{z^{\max}_{\text{sink in interval 1}}} = \Delta G_1 \tag{3.7}$$

where F_1^{Sink} is the flowrate required by the sinks in interval 1

For feasibility to be attained in the first interval, there exist δ_1 such that

$$F_1^{Sources} + \delta_1^{'} \geq F_1^{Sink} \tag{3.8}$$

where $\delta_1^{'} \geq 0$.

At M_2 and ΔM_2:

$$F_2^{Sources} = F_1^{Sources} + \frac{\Delta M_2}{y_{\text{source in interval 2}}} = \Delta W_1 + \Delta W_2 = \sum_{n=1}^{2} \Delta W_n \tag{3.9}$$

where $F_2^{Sources}$ is the total flowrate of the sources that is available for use to the sinks up to interval 2

$$F_2^{Sink} = F_1^{Sink} + \frac{\Delta M_2}{z_{\text{sink in interval 2}}^{\max}} = \Delta G_1 + \Delta G_2 = \sum_{n=1}^{2} \Delta G_n \tag{3.10}$$

where F_2^{Sink} is the total flowrate required by the sinks up to interval 2

For feasibility to be attained in the second interval, there exists $\delta_2^{'}$ such that

$$F_2^{Sources} + \delta_2^{'} \geq F_2^{Sink} \tag{3.11}$$

where $\delta_2^{'} \geq 0$.

Similarly, at any interval k with load M_k and load interval ΔM_k:

$$F_k^{Sources} = \frac{\Delta M_k}{y_{\text{source in interval } k}} + \sum_{n=1}^{k-1} \Delta W_n = \sum_{n=1}^{k} \Delta W_n \tag{3.12}$$

where $F_k^{Sources}$ is the total flowrate of the sources that is available for use to the sinks up to interval k.

$$F_k^{Sink} = \frac{\Delta M_k}{z_{\text{sink in interval } k}^{\max}} + \sum_{n=1}^{k-1} \Delta G_n = \sum_{n=1}^{k} \Delta G_n \tag{3.13}$$

where F_k^{Sink} is the total flowrate required by the sinks up to interval k

For feasibility to be attained in the k^{th} interval, there exists $\delta_k^{'}$ such that

$$F_k^{Sources} + \delta_k^{'} \geq F_k^{Sink} \tag{3.14}$$

where $\delta_k^{'} \geq 0$.

In case there is deficit amount of process resources within interval k, then $\delta_k^{'}$ amount of fresh sources must be supplied to that interval in order to insure feasibility.

3.5 Algebraic Targeting Procedure for Pure Fresh Resources

First, we derive the algebraic procedure for the case when the fresh source is pure. As seen in Figure 3.3, for any given load the sink composite curve must lie to the left of the source composite curve so as not to have a shortage of the flow necessary for the sinks as described in the feasibility conditions stated above. The most negative number of all δ's (which is designated as $\delta_{\max}$) constitutes the maximum shortage of flowrate and corresponds to the minimum usage of fresh source. By horizontally sliding the source composite curve to the right by a distance equal to $\delta_{\max}$ (Figure 3.4), we eliminate all infeasibilities. Consequently, the target for minimum fresh usage is equal to the maximum shortage, i.e.

$$\text{Target for Minimum Fresh Consumption } = \left|\delta_{\max}\right| = \delta_0^{'} \qquad (3.15)$$

In order to develop the algebraic procedure, it is necessary to evaluate this maximum shortage algebraically. Towards this end, the feasibility conditions stated above will be utilized by changing the inequalities of flows into equalities for each interval, i.e.

$$F_k^{Sources} + \delta_k^{'} = F_k^{Sink} \qquad (3.16)$$

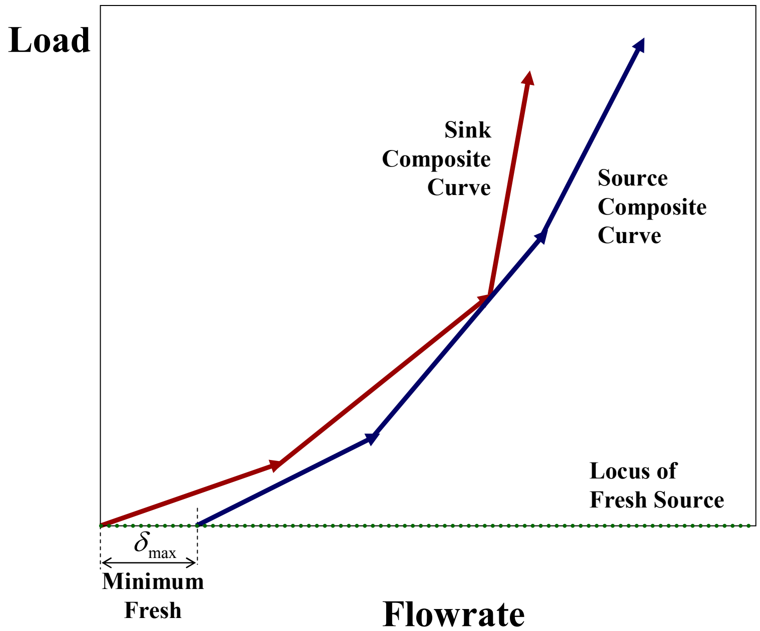


Figure 3.4 Minimum fresh target for pure fresh resources.

We define a positive δ_k as a surplus and a negative δ_k as a deficit (corresponding to infeasibility). Substituting Equations (3.12) and (3.13) into Equation (3.16) and re-arranging, we get

$$\delta_k = \sum_{n=1}^{k} \Delta W_n - \sum_{n=1}^{k} \Delta G_n \tag{3.17}$$

This expression may be verified from Figure 3.3 by applying it to intervals 1 and 2, respectively, to get:

$$\delta_1 = \Delta W_1 - \Delta G_1 \tag{3.18}$$

and

$$\delta_2 = \Delta W_1 + \Delta W_2 - \Delta G_1 - \Delta G_2 \tag{3.19}$$

Substituting Equation (3.18) into Equation (3.19), we obtain

$$\delta_2 = \delta_1 + \Delta W_2 - \Delta G_2 \tag{3.20}$$

and, for the k^{th} interval, we have

$$\delta_k = \delta_{k-1} + \Delta W_k - \Delta G_k \tag{3.21}$$

with $\delta_0 = 0$. Equation (3.21) is represented by Figure 3.5. The flow balances can be carried out for all intervals resulting in the cascade diagram shown in Figure 3.6. In the cascade diagram, the most negative value of δ (referred to as $\delta_{\max}$) corresponds to the target for minimum fresh consumption as indicated by Equation (3.15) and the amount of waste is equal to the sum of $\delta_{\bar{k}}$ and $|\delta_{\max}|$. Additionally, in order to remove the infeasibilities a flowrate of the fresh resource equal to $|\delta_{\max}|$ is added to the top of the cascade (i.e., $\delta_0^{'} = |\delta_{\max}|$) and the residuals of all intervals are adjusted, thus eliminating all the infeasibilities. The result is that the most negative residual now becomes zero indicating the pinch location. Furthermore, the revised residual leaving the last interval is the target for minimum wastewater discharge. These results are shown on the revised cascade diagram illustrated in Figure 3.7.

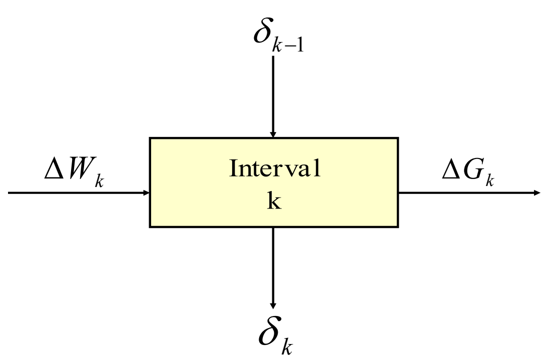


Figure 3.5 Flow balance around a load interval for impure fresh resources.

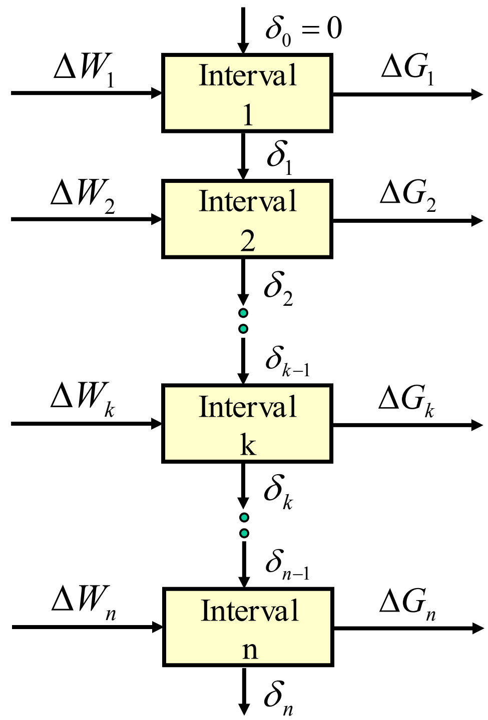


Figure 3.6 Cascade diagram for impure fresh resources.

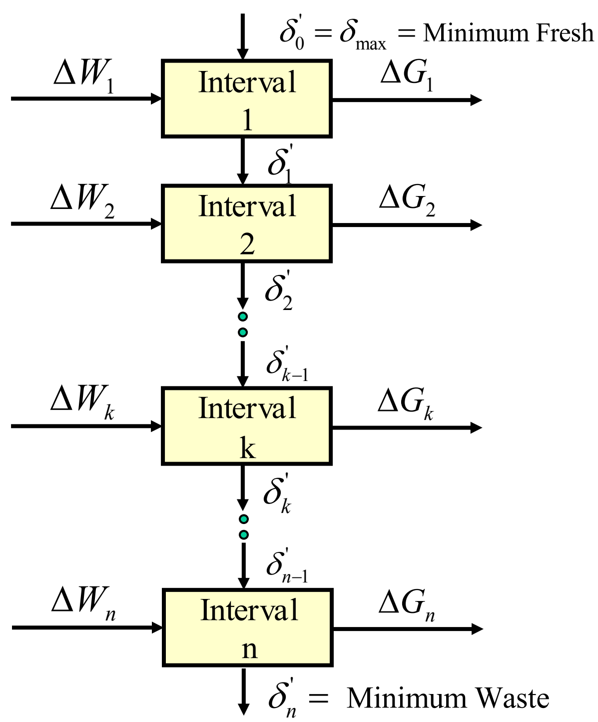


Figure 3.7 Revised cascade diagram for impure fresh resources.

3.6 Algebraic Targeting Procedure for Impure Fresh Resources

Next, we generalize the algebraic procedure to address the more general case of using impure fresh sources. Figure 3.8 is the more general representation of Figure 3.4 where the source composite curve is slid on the fresh locus (having a slope of the composition of impurities).

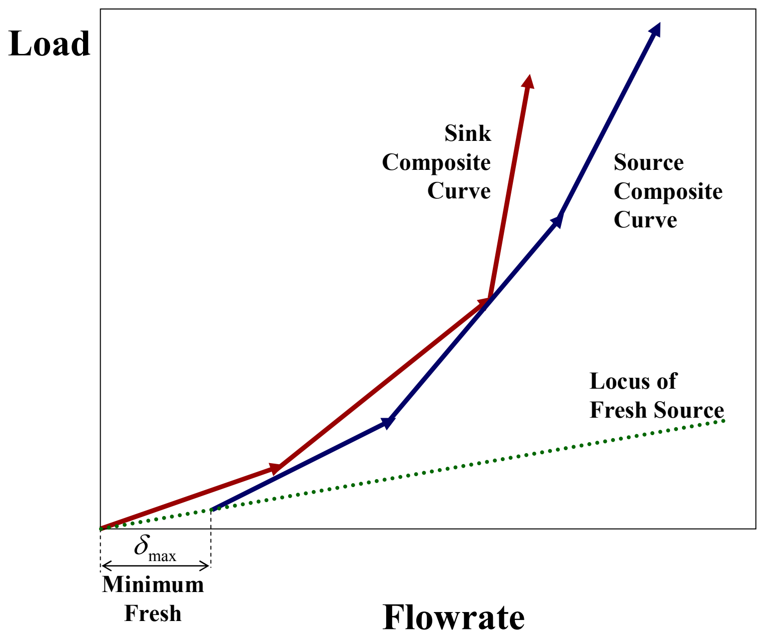


Figure 3.8 Minimum fresh target for impure fresh sources.

To develop the algebraic procedure for the case shown in Figure 3.8, we propose the following alternatives:

Change the coordinate system by rotating the flowrate-axis anti-clockwise by a degree (θ), so that it coincides with the fresh feed locus as shown in Figure 3.9, where

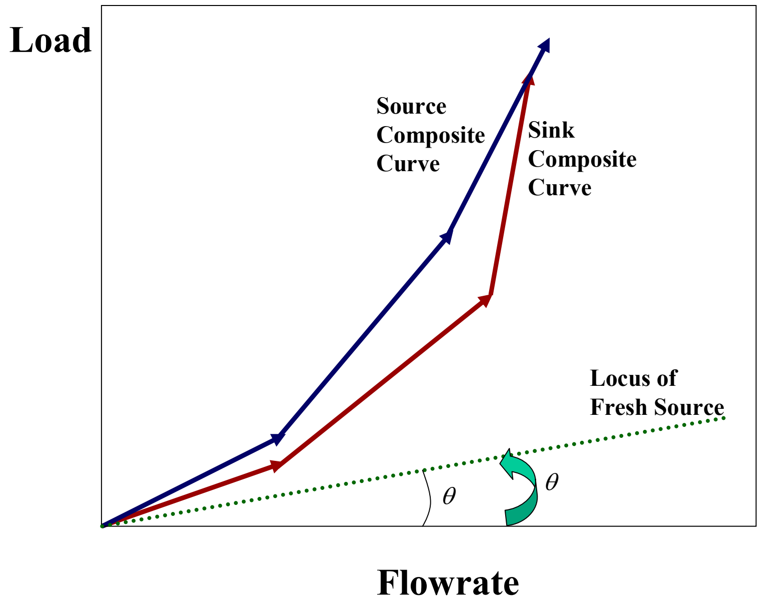


Figure 3.9 Rotation of composite curves by the angle of fresh resources locus.

$$\theta = \tan^{-1} y_f \tag{3.22}$$

Towards this end, we need to account for a respective change in the flowrates and contaminant concentrations for all the components of the system according to the following Equations (3.23)–(3.28), as shown in Figure 3.9

$$G' = G\cos\theta \tag{3.23}$$

Similarly,

$$W' = W\cos\theta \tag{3.24}$$

and

$$Y_i = y_i - y_f \tag{3.25}$$

$$Z_j^{\max} = z_j^{\max} - y_f \tag{3.26}$$

Then, the corresponding loads for sinks and sources are the following:

$$M_i^{'} = W_i^{'} \, Y_i \tag{3.27}$$

$$M_j^{'} = G_j^{'} \, Z_j^{\max} \tag{3.28}$$

The target for minimum fresh source consumption and waste discharge are brought back to the old coordinate through:

Target for Minimum Fresh Consumption $= \delta_0^{'} / \cos(\theta)$

and

Target for Minimum Waste Discharge $= \delta_n^{'} / \cos(\theta)$

The same outcome is obtained by rotating the system clockwise, so as the fresh locus coincides with the flowrate-axis of the new coordinate systems.

An alternate method involves the adjustment of the load contribution of the fresh feed on both composites as shown in Figure 3.10. The load contribution of the fresh is the product of its flowrate and composition and, therefore, may be readily calculated. In this case, the residuals (including $\delta_{\max}$ or the target for minimum fresh consumption) may be calculated by first determining ΔW_k and ΔG_k for any interval k and then using Equations (3.17) or (3.21) for residual balance The goal is to generate an equation that eliminates the use of the fresh flowrate and/or the fresh load, since these are the unknown variables in the problem.

According to Equation (3.3) and Figure 3.10, ΔM_k may be regarded as the total load within interval k, which incorporates both the load of the source and the load of the fresh in interval k. Thus, ΔW_k is given by:

$$\Delta W_k = \Delta M_k^{tot} / y_{i,k} = (M_k^{tot} - M_{k-1}^{tot}) / y_{i,k} \tag{3.29}$$

or

$$\Delta W_k = [(M_k + M_{fr,k}) - (M_{k-1} + M_{fr,k-1})] / y_{i,k}$$

$$\Delta W_k = (M_k - M_{k-1}) / y_{i,k} + (M_{fr,k} - M_{fr,k-1}) / y_{i,k} \tag{3.30}$$

where M_k and M_{k-1} are now the loads contributed purely from the source in intervals k and $k-1$ respectively, whereas $M_{fr,k}$ and $M_{fr,k-1}$ are the load of the fresh in interval k and $k-1$ respectively, as seen in Figure 3.10. Next, Equation (3.30) can be transformed to Equation (3.31) by eliminating the load contributions of the fresh:

$$\Delta W_k = (M_k - M_{k-1}) / y_{i,k} + \Delta W_k y_{fr} / y_{i,k} \tag{3.31}$$

since

$$\Delta W_k = (M_{fr,k} - M_{fr,k-1}) / y_{fr} \tag{3.32}$$

Thus, Equation (31) takes the following form:

$$\Delta W_k = (M_k - M_{k-1}) / (y_{i,k} - y_{fr}) = \Delta M_k / (y_{i,k} - y_{fr}) \tag{3.33}$$

Similarly, ΔG_k is given by:

$$\Delta G_k = \Delta M_k / (z_{j,k}^{\max} - y_{fr}) \tag{3.34}$$

Now that the flows, loads, and residuals have been transformed to take the same shape as in the case of targeting with pure fresh, the algebraic procedure for impure fresh follows the same rules as in the case of pure fresh, when considering Equations (3.25)-(3.28) for calculating the flows, the compositions, and the loads.

Thus, the loads of sources and sinks are now given by the following equations:

$$M_i = W_i \, Y_i \tag{3.35}$$

$$M_j = G_j \, Z_j^{\max} \tag{3.36}$$

where

$$Y_i = y_i - y_f \tag{3.37}$$

$$Z_j^{\max} = z_j^{\max} - y_f \tag{3.38}$$

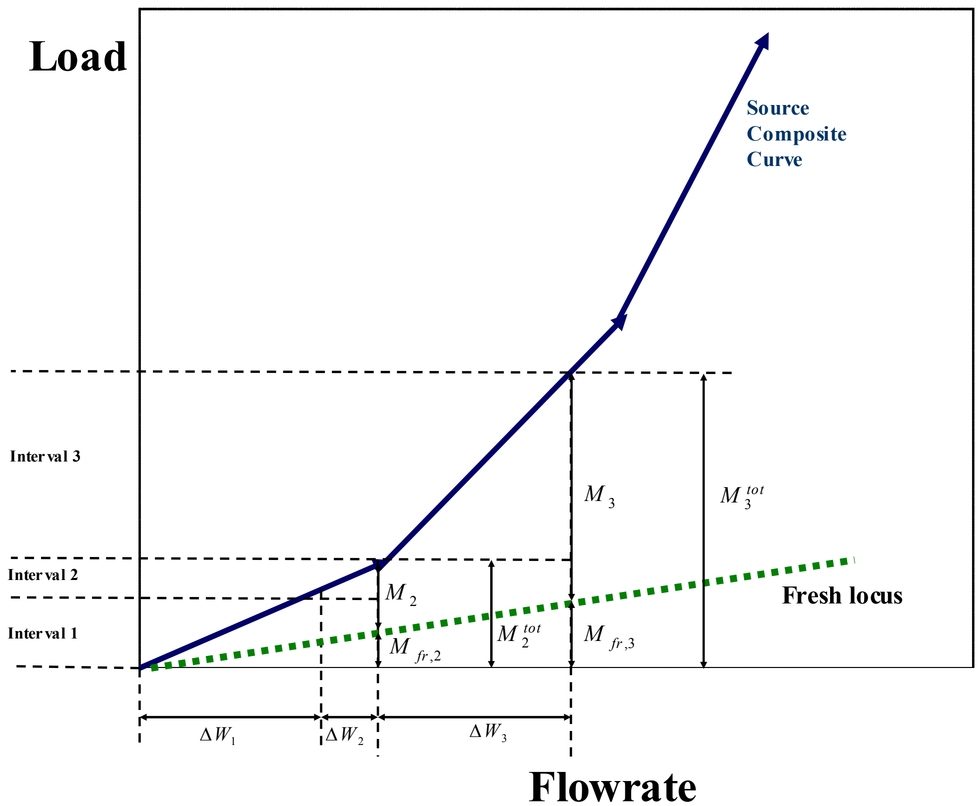


Figure 3.10 Elimination of fresh source contribution from source composite curve.

In this work, we will concentrate on the last method to tackle non-pure fresh resource cases. In doing so, the concept of pure fresh resource mentioned earlier is applied.

Another obstacle is the presence of a process source that is purer than the fresh source as shown in Figure 3.11. In such a case, the source prioritization rule is applied to every process source that is purer than the fresh source prior to applying the method, thus splitting the problem into two sub-problems; one before the introduction of fresh sources and one after.

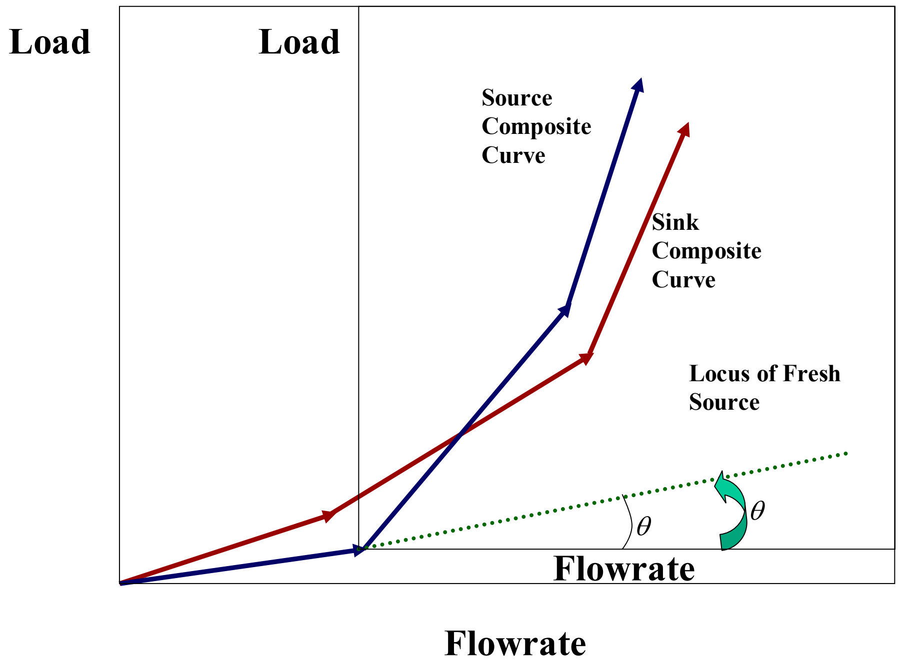


Figure 3.11 Case when process source is purer than fresh source.

Based on the foregoing analysis, the algebraic procedure can be summarized as follows:

1. Rank the sinks in ascending order of maximum admissible composition, $z_1^{\max} \leq z_2^{\max} \leq \ldots z_j^{\max} \ldots \leq z_{N_{Sinks}}^{\max}$
2. Rank sources in ascending order of pollutant composition, i.e. $y_1 < y_2 < \ldots y_i \ldots\ldots < y_{N_{Sources}}$
3. If necessary, apply the source prioritization rule for all sources i, whose pollutant compositions are $y_i \leq y_f$ and eliminate them from the ranking, as well as for all

sinks with flowrates that have been satisfied by those eliminated sources, such that

$$\sum_{i=1}^{N_{sources}} W_i - \sum_{j=1}^{N_{sinks}} G_j = 0 \quad \forall i : y_i \leq y_f$$

4. If necessary, eliminate the fresh source load contribution by subtracting the contaminant concentration from that of sources and sinks as follows

$$Y_i = y_i - y_f$$

$$Z_j^{\max} = z_j^{\max} - y_f$$

5. Calculate the load of each sink ($M_j^{Sink,max} = G_j\, Z_j^{max}$) and source ($M_i^{Source} = W_i Y_i$).
6. Compute the cumulative loads for the sinks and for the sources (by summing up their individual loads).
7. Rank the cumulative loads in ascending order.
8. Develop the load-interval diagram (LID) shown in Figure 3.12. First, the loads are represented in ascending order starting with a zero load. The scale is irrelevant. Next, each source (and each sink) is represented as an arrow whose tail corresponds to its starting load and head corresponds to its ending load. Equations (3.3)-(3.5) are used to calculate the intervals load, source flowrate, and sink flowrate.
9. Based on the interval source- and sink flowrates, develop the cascade diagram and carry out flow balances around the intervals to calculate the values of the flow residuals (δ_k's). The most negative δ_k is the target for minimum fresh consumption.

10. Revise the cascade diagram by adding the maximum $|\delta_{\max}|$ to the first interval and calculate the revised residuals. The residual flow leaving the last interval is the target for minimum waste discharge. The interval with the first zero residual is the material recycle/reuse global pinch point.

It is worth mentioning that the procedure is also valid for pure fresh resources, by simply setting $y_f = 0$ (or equivalently $\theta = 0$) and sliding the source composite curve along the flowrate locus itself.

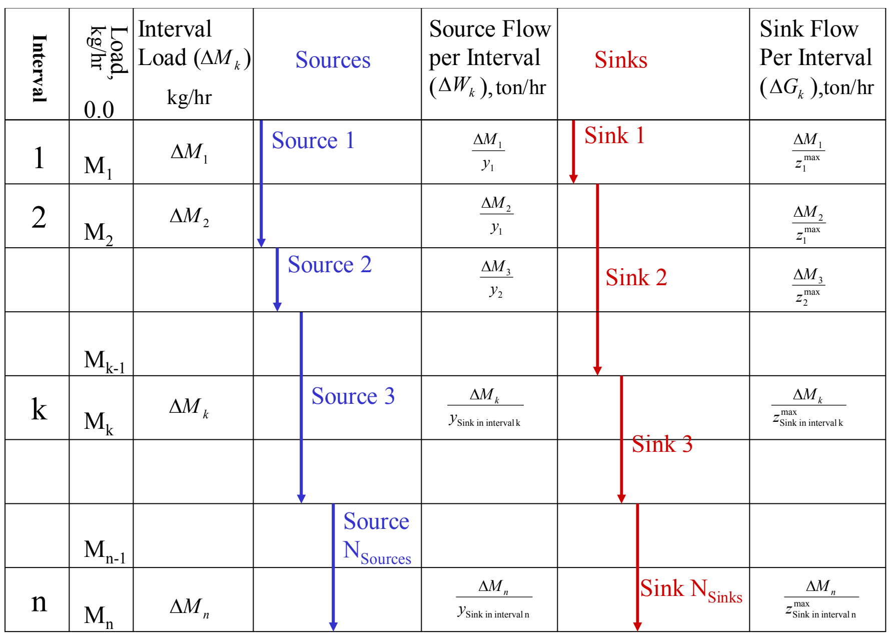


Figure 3.12 Load interval diagram.

3.7 Case Studies

In the following examples, we illustrate the merit, rigor, and applicability of the developed method.

Example 1. This case study is taken from Alves and Towler (2002) for the optimization of a hydrogen distribution system within a refinery; it is comprised of four sinks and six sources. The pertinent information regarding these sinks and sources are shown in Table 3.1. Additionally, in this case study the fresh resource contains a small quantity of impurity, i.e. the fresh hydrogen at a 5% impurity level.

Table 3.1 Alves and Towler (2002) case study information.

Sinks	**Flow, mol/s**	$z_j^{\max}$ **mol%**	$Z_j^{\max}$ **mol%**	**Load, mol/s**	**Cumulative Load, mol/s**
1	2495	19.39	14.39	359.03	359.03
2	180.2	21.15	16.15	29.10	388.13
3	554.4	22.43	17.43	96.63	484.76
4	720.7	24.86	19.86	143.13	627.90
Sources	**Flow, mol/s**	y_i **mol%**	Y_i **mol%**	**Load, mol/s**	**Cumulative Load, mol/s**
1	623.8	7	2	12.48	12.48
2	415.8	20	15	62.37	74.85
3	1801.9	25	20	360.38	435.23
4	138.6	25	20	27.72	462.95
5	346.5	27	22	76.23	539.18
6	457.4	30	25	114.35	653.53

Using the information in Table 3.1, the LID is generated and shown in Figure 3.13. The cascade diagram is given by Figure 3.14(a). As can be seen, the most negative residual is –268.82 mols/s. Therefore, the target for minimum fresh hydrogen is 268.82 mols/s. Adding this value to the first interval, the revised cascade calculations are carried out leading to a target of minimum hydrogen discharge (residual leaving last interval) of 102.52 mols/s. The pinch location is at the zero residual. Hence, the material recycle pinch point is located at the horizontal lines separating intervals 9 and 10 corresponding to a source composition of 30%. These values are in agreement with those found by Alves and Towler (2002) using the iterative Hydrogen Surplus Diagram approach.

Interval	Load mol/s 0.0	Interval Load (ΔM_k) kmol/hr	Sources	Source Flow Per Interval (ΔW_k), kmol/hr	Sinks	Sink Flow Per Interval (ΔG_k), kmol/hr
1	12.48	12.48	Source 1 Y=0.02	623.80		86.7
2	74.85	62.37	Source 2 Y=0.15	415.80	Sink 1 Z^{max}=0.1439	433.43
3	359.03	248.18		1420.92		1974.87
4	388.13	29.20	Source 3 Y=0.20	145.51	Sink 2 Z^{max}=0.1615	180.20
5	435.23	47.09		235.47		270.18
6	462.95	27.72	Source 4 Y=0.20	138.60	Sink 3 Z^{max}=0.1743	159.04
7	484.76	21.82	Source 5 Y=0.22	99.18		125.18
8	539.18	54.41		247.32	Sink 4 Z^{max}=0.1986	273.97
9	627.90	88.72	Source 6 Y=0.25	354.88		446.73
10	653.53	25.63		102.52		0

Figure 3.13 LID for Alves and Towler case study.

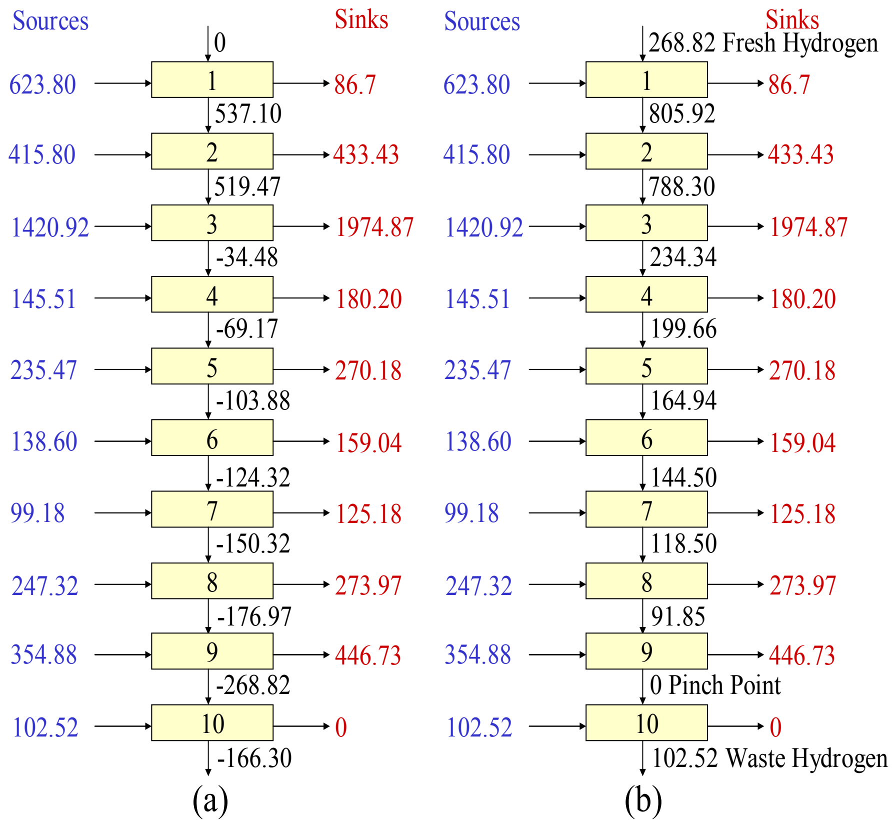


Figure 3.14 Cascade diagram for Alves and Towler case study, (a) with infeasibilities (b) revised.

Example 2. The presence of purer process sources than the fresh source is explored next. Lovelady et al. (2005) presented a case study for a pulp and paper mill with data presented in Table 3.2. Fresh water is available at a chloride concentration of 3.7 ppm.

A schematic diagram of the process is shown in Figure 3.15. The source prioritization rule is applied and the problem is split into two sub-problems. One involves sources purer than the fresh source, and the other deals with sources less clean than the fresh source.

Table 3.2 Source-sink information for Lovelady case study (Lovelady, 2002).

Sinks	Flow, ton/day	$z_j^{\max}$, ppm	Load, kg/day
1	1450	4.5	6.525
2	13995	6.8	95.166
Sources	**Flow, ton/day**	y_i, **ppm**	**Load, kg/day**
1	8901	0	0
2	10995	35.8	393.621

Sub-Problem 1. Examining Table 3.2 reveals that Source 1 contaminant concentration is zero which is cleaner than the fresh source. Therefore, the first source flow (W_1) is totally exploited prior to considering the addition of the fresh source. The sink flow or portion of it being fulfilled by W_1 is such that

$$W_1 - \sum_{j=1}^{N_{sinks}} G_j = 0$$

Since $W_1 > G_1$ and $W_1 - G_1 < G_2$, then the first sink flow requirement will be totally fulfilled and sink 2 flow needs is partially fulfilled by the remaining flow of source 1.

$$G_2^{'} = G_2 - (W_1 - G_1) = 13995 - (8901 - 1450) = 6544\, ton/day$$

Therefore, only 6544 ton/day of sink 2 should be satisfied by other sources. The load that has been removed from sink 1 and portion of sink 2 is

$$M = G_1\, z_1^{\max} + (W_1 - G_1)\, z_2^{\max} = (1450 \cdot 4.5 - (8901 - 1450) \cdot 6.8) \cdot 10^{-3} = 57.192\, kg/day$$

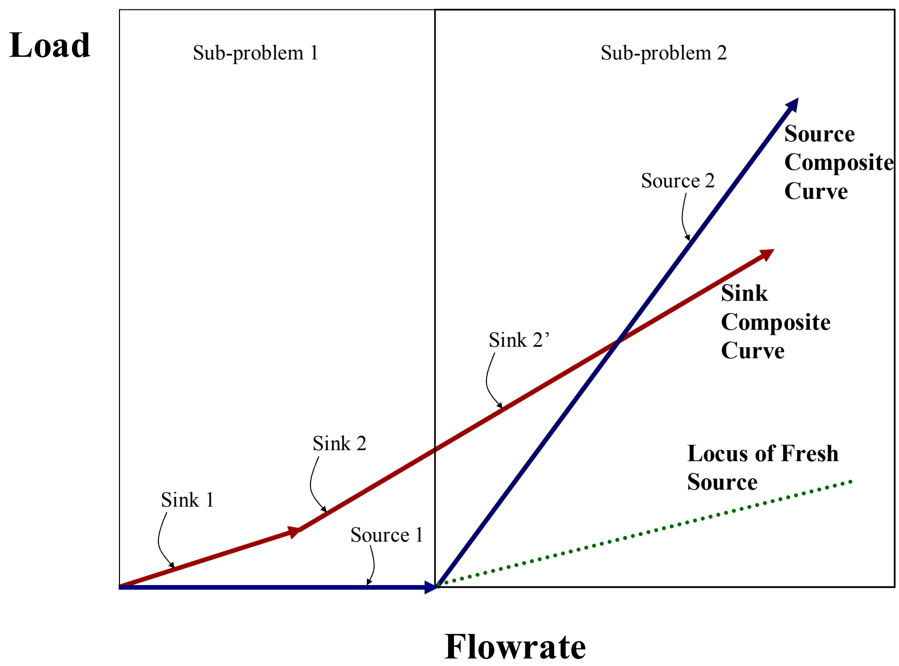


Figure 3.15 Schematic diagram for example 2.

Sub-Problem 2. Table 3.2 is revised to incorporate the second sub-problem only, as shown in Table 3.3. To establish a systematic way for the targeting procedure, a fictitious sink is added at the beginning to account for the load starting point for the second sink as shown in Figure 3.15. The individual load for each sink and source in the process is calculated and cumulative loads are obtained as shown in Table 3.3. The cumulative load for the whole process is then arranged in ascending order to obtain the number of intervals followed by calculating the flowrates of the sinks and sources through each interval as shown in Figure 3.16. Using L'Hopital's rule for the first interval, sink flowrate can be determined as shown below:

$$\Delta G_1 = \frac{\Delta M_1}{Z_{1\text{in interval }1}^{\max}} = \frac{d(\Delta M_1)}{d(Z_{1\text{in interval }1}^{\max})} = G_{1'} \tag{3.39}$$

Table 3.3 Revised source-sink information for Lovelady case study.

Sinks	**Flow, ton/day**	$z_j^{\max}$, **ppm**	$Z_j^{\max}$, **ppm**	**Load kg/day**	**Cumulative Load, kg/day**
1’	0	3.7	0	57.192	57.192
2’	6544	6.8	3.1	20.286	77.478
Sources	**Flow, ton/day**	y_i, **ppm**	Y_i, **ppm**	**Load kg/day**	**Cumulative Load, kg/day**
2	10995	35.8	32.1	352.94	352.94

Once the LID table is established, the cascade diagram is set up with the relevant flowrates of sinks and sources through each interval. The most negative residual value in the cascade diagram indicates the minimum amount of fresh water must be supplied to the process, as can be seen from Figure 3.17 the minimum freshwater is 4130.35 ton/day and the minimum wastewater discharge is 8581.35 ton/day. These values conform to solution obtained by linear programming module.

Interval	Load kg/day 0.0	Interval Load (ΔM_k) kg/day	Sources	Source Flow Per Interval (ΔW_k), ton/day	Sinks	Sink Flow Per Interval ΔG_k, ton/day
1	57.192	57.192	Source 2 Y=32.1	1781.68		0
2	77.478	20.286		631.98	Sink 2' Z^{max}=3.1	6544
3	352.94	275.461		8581.35		0

Figure 3.16 LID for Lovelady case study.

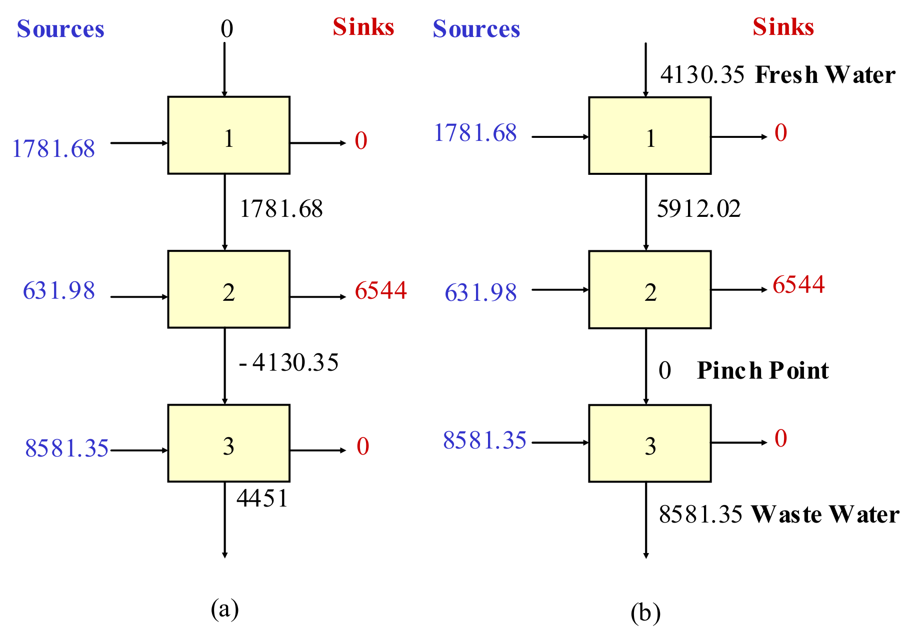


Figure 3.17 Cascade diagram for Lovelady case study, (a) with infeasibilities (b) revised.

3.8 Conclusions

In this chapter we introduced a systematic algebraic procedure for the targeting of material-recycle networks. Based on the visualization tool of material-recycle pinch analysis, analogous algebraic constraints were derived. These constraints along with the optimality conditions were used to develop a cascade analysis. The cascade diagram calculations result in the identification of rigorous targets on the minimum usage of fresh source and the minimum discharge of waste. By rotating the composite representation for sources and sinks, the algebraic procedure is generalized to the cases when impure fresh sources are used. Two case studies were solved to illustrate the applicability of the devised procedure.

3.9 Nomenclature

G Sink (unit) flow, mass or volume/time

M Load, mass or volume/time

$N_{sources}$ Number of process streams (or sources)

N_{sinks} Number of process units (sinks)

W Sink (unit) flow, mass or volume/time

y Contaminant composition of process streams (or sources)

z Allowable contaminant composition of process unit (or sink)

$\bar{k}$ Total number of intervals

Superscripts

min Unit (sink) lower bound of allowable contaminant concentration

max Unit (sink) upper bound of allowable contaminant concentration

Subscripts

i Index for sources

j Index for sinks

k Interval index

Greek Letters

δ Interval Residual, mass or volume/time

Δ Difference between two consecutive intervals

CHAPTER IV

ALGEBRAIC PROPERTY TARGETING FOR FRESH RESOURCES

4.1 Literature Review

Primarily, process design and integration has always been approached by the use of component balances. Tracking of individual species has always been the heart of any design approach. Even though much progress has been made through the years in the field of design and optimization, a more intuitive approach has been developed that targets properties as the basis for integration. Shelley and El-Halwagi (2000) introduced the concept of component-less design based on tracking properties through dimensionless conserved quantities known as clusters that are based on property mixing rules. Eden et al. (2002) addressed the problem of simultaneous process and molecular design by using the clustering concept for property-based representations. Optimal property profiles for candidate fresh resources were obtained, and computer-aided molecular design techniques were used to yield fresh resources with the desired property profiles (reverse problem formulation). Gani and Pistikopoulos (2002) also discussed the role of property-based models in the design of product and processes. Two approaches were developed; one used a mixed-integer nonlinear optimization model for property-based product and process design and simulation, whereas the other employed reduction techniques to lump thermodynamic variables for graphical solutions. Property-based models for separation applications were investigated by Eden et al. (2004). El-Halwagi et al. (2004) derived cluster-based lever arm optimization rules to foster material reuse using graphical representations, whereas a new algebraic technique for optimal resource allocation in a component-less mode was developed by Qin et al. (2004).

4.2 Problem Statement

Given is a process with a number, $N_{sources}$ of streams (sources) that can be considered for possible reuse and replacement of the fresh material. Each source, i, has a given flowrate, W_i, and a given property value, p_i. These sources can be utilized in a number, N_{sinks} of process units (sinks). Each sink, j, requires a feed with a given flowrate, G_j, and an inlet property, p_j^{in}, that satisfies the following constraint:

$$p_j^{\min} \le p_j^{in} \le p_j^{\max} \qquad j = 1, \cdots, N_{sinks} \tag{4.1}$$

Available for service is a fresh (external) resource whose property value is p_{Fresh} and can be purchased to supplement the use of process sources in sinks.

The objective is to develop a non-iterative algebraic approach that determines the target for minimum usage of the fresh resource, maximum material reuse and minimum discharge to waste.

4.3 Problem Formulation Background

In order to track properties throughout a process, the basic equations from Shelley and El-Halwagi (2000) are used. The mixing rule for a given property is described by:

$$\psi(\bar{p}) = \sum_i x_i \psi(p_i) \tag{4.2}$$

where $\psi(p_i)$ and $\psi(\bar{p}_i)$ are operators on property p_i and mixture property $\bar{p}_i$ respectively; x_i is the fractional contribution of source i into the total flowrate of the mixture, i.e.

$$x_i = \frac{F_i}{\sum_i F_i} \tag{4.3}$$

Equation (4.2) is arranged in such a way that the weighted average summation of the operators on individual properties will yield the operator on the mean property of the mixture. Numerous properties can be expressed using this general linear mixing rule in Equation (4.2). One example would be the mixing of different sources with individual density ρ_i to form a mixture with mean density $\bar{\rho}$. The mixing rule for density follows Equation (4.4):

$$\frac{1}{\bar{\rho}} = \sum_i \frac{x_i}{\rho_i} \tag{4.4}$$

If we compare Equation (4.4) with the general rule of property mixing (Equation (4.2)), we conclude that the operator for density is given as:

$$\psi(\rho_i) = \frac{1}{\rho_i} \tag{4.5}$$

Equation (4.2) can be applied to a wide rage of properties having different patents of mixing rule. Operators for other product-related properties (e.g. RON number for oil mixture, miscibility for liquids, etc.) that follow the general mixing rule in Equation (4.2) can also be defined in a similar way. For simplicity, $\psi(\rho_i)$ will be referred as ψ in the remainder of the text.

Having defined the general rule for deriving an operator for a given property, the sink constraints in Equation (4.1) can be rewritten using the new definition of operator, as follows:

$$\psi_j^{\min} \leq \psi_j^{in} \leq \psi_j^{\max} \qquad j = 1, \cdots, N_{sinks} \tag{4.6}$$

Although there is an upper and a lower bound of the operator constraints in Equation (4.6), only one of these bounds will be used as the *limiting data* in any network synthesis problem. The concept of the limiting data will be further described when the example is introduced in the later sections of this chapter.

Next, another important parameter needs to be defined in property integration. This is the so-called *property load M*, which is the product of the flowrate of a source (W_i) or sink (G_j) with its associated property operator (ψ_i and ψ_j respectively). The property loads for a source *i*, M_i and a sink *j*, M_j are given in Equation (4.7) and Equation (4.8) respectively:

$$M_i = W_i \Psi_i \tag{4.7}$$

$$M_j = G_j \Psi_j \tag{4.8}$$

This newly defined parameter provides information that resembles the information given by the mass load in the conventional mass integration approach presented in the previous two chapters. Note that the property of a sink is always bounded within a range of properties or its associated operators. Consequently, due to the constant flowrate required by a sink, the constraints of the sink in Equation (4.6) can be rewritten in terms of property load as shown in Equation (4.9):

$$M_j^{\min} \leq M_j^{in} \leq M_j^{\max} \qquad j = 1, \cdots, N_{sinks} \tag{4.9}$$

Equation (4.9) implies that when feeding a process source to a process sink, its property load should not fall beyond the range of property loads, which are acceptable by the sink. Therefore, Equation (4.9) replaces the constraints imposed when feeding process source(s) to a sink.

To this end, the approach for material recycle/reuse presented in chapter 3 is applicable for all facets of property integration discussed earlier. Therefore, we are in a position now to proceed to the case studies.

4.4 Case Studies

In the following examples, we illustrate the merit, rigor, and applicability of the developed method.

Example 1. This case study pertaining to metal degreasing process is taken from Shelley and El-Halwagi, (2000). The process is comprised of two sinks and two sources. The pertinent information regarding these sinks and sources are shown in

Table 4.1. The fresh resource Reid vapor pressure is given in the table as well.

The adjusted operator for both sources and sinks to account for the load contribution of the fresh source property is obtained via the following equations

$$\Psi_i = \psi_i - \psi_{Fresh} \tag{4.10}$$

$$\Psi_j = \psi_j - \psi_{Fresh} \tag{4.11}$$

Individual loads are calculated according to Equations (4.7) and (4.8), cumulative loads are then evaluated as shown in Table 4.2. Using the information in Table 4.2, the LID is generated and shown in Figure 4.1. The cascade diagram is depicted by Figure 4.2(a). As can be seen, the most negative residual is –2.38 kg/s. Therefore, the target for minimum fresh solvent is 2.38 kg/s. Addition of this value to the first interval and revising cascade calculations leads to a target of minimum hydrogen discharge (residual leaving last interval) of 2.38 kg/s. The pinch location is at the zero residual. Hence, the material recycle pinch point is located at the horizontal lines separating intervals 3 and 4 corresponding to a source property value of 10.49 or RVP of 6 psi.

Table 4.1 Sources and sinks information for Shelley and El-Halwagi case study (Shelley and El-Halwagi, 2000).

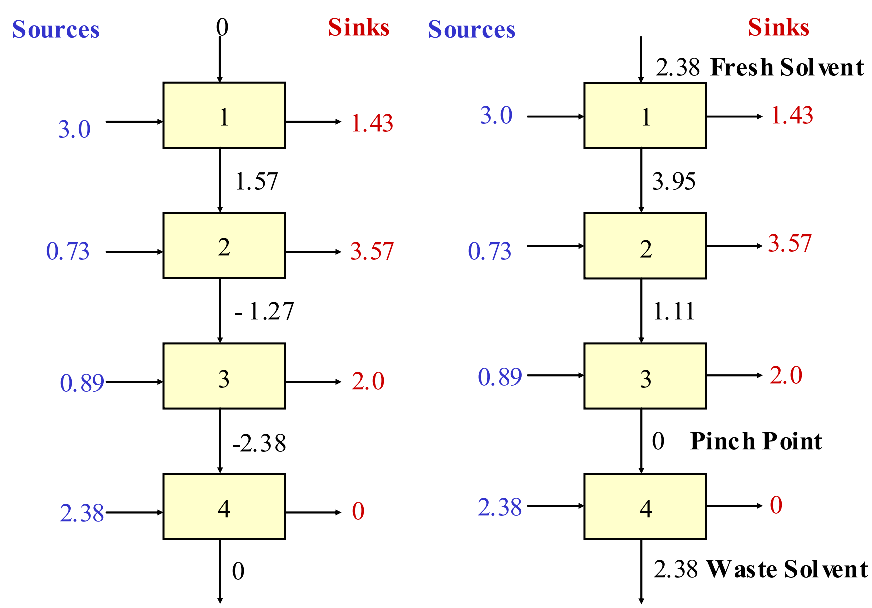
Sink	**Flowrate, kg/s**	**RVP, psi**	**Operator** $\psi = RVP^{1.44}$
1	5	3	4.86
2	2	4	7.36
Sources	**Flowrate, kg/s**	**RVP, psi**	**Operator** $\psi = RVP^{1.44}$
Fresh	-	2	2.71
1	3	2.5	3.74
2	4	6	13.20

Table 4.2 Sources and sinks cumulative load for Shelley and El-Halwagi case study.

Sink	**Flowrate, kg/s**	**Operator** Ψ	**Load, kg/s**	**Cumulative Load, kg/s**
1	5	2.15	10.75	10.75
2	2	4.65	9.30	20.05
Sources	**Flowrate, kg/s**	**Operator** Ψ	**Load, kg/s**	**Cumulative Load, kg/s**
1	3	1.03	3.09	3.09
2	4	10.49	41.94	45.03

Interval	Load kg/s 0.0	Interval Load (ΔM_k) kg/s	Sources	Source Flow per Interval (ΔW_k), kg/s	Sinks	Sink Flow per Interval (ΔG_k), kg/s
1	3.0	3.09	Source 1 Ψ =1.03	3.00	Sink 1 Ψ^z=2.15	1.43
2	10.7	7.66		0.73		3.57
3	20.0	9.30	Source 2 Ψ =10.49	0.89	Sink 2 Ψ=4.65	2.00
4	45.0	24.98		2.38		

Figure 4.1 LID for Shelley and El-Halwagi case study.



(a) (b)

Figure 4.2 Cascade diagram for Shelley and El-Halwagi case study, (a) with infeasibilities (b) revised.

Example 2. A papermaking process is presented in this case study (2004). The objective of this case study is to explore the possibilities of recycling and reusing the waste streams, thus reducing the fresh source consumption and maximizing the resource usage.

Reflectivity, defined as the reflectance of an infinitely thick material compared to an absolute standard, is used to evaluate the quality of the broke to be used as a feed stream to the sinks. The mixing rule for reflectivity R is of the following form El-Halwagi et al. (2004):

$$\overline{R}^{5.92} = \sum_{i=1}^{N} x_i R_i^{5.92} \tag{4.12}$$

Table 4.3provides the data for the property constraints of the sinks and the properties of the process sources and the fresh, along with their flow rates.

Table 4.3 Source-sink information for papermaking example (El-Halwagi et al. 2004)).

Sink	**Flowrate ton/hr**	**Reflectivity R**	**Operator $\psi = R^{5.92}$**
1	40	0.9	0.54
2	100	0.85	0.38
Source	**Flowrate ton/hr**	**Reflectivity R**	**Operator $\psi = R^{5.92}$**
Fresh		0.95	0.74
1	90	0.88	0.47
2	60	0.75	0.18

As can be seen from Table 4.3, the reflectivity (operator) of the fresh feed is higher than that of sources and sinks. The treatment of the problem is not different from the previous one except that the adjusted operator will be negative for the process and consequently the load.

The individual load for each sink and source in the process is calculated and cumulative loads are obtained as shown in Table 4.4. The cumulative load for the whole process is then arranged in ascending order to obtain the number of intervals followed by calculating the flowrates of the sinks and sources through each interval as shown in Figure 4.3.

Table 4.4 Cumulative load of sources and sinks for papermaking example.

Sink	**Flowrate, ton/hr**	**Operator Ψ**	**Load, ton/hr**	**Cumulative Load, ton/hr**
1	40	-0.20	-8.09	-8.09
2	100	-0.36	-35.60	-43.69
Source	**Flowrate, ton/hr**	**Operator Ψ**	**Load, ton/hr**	**Cumulative Load, ton/hr**
1	90	-0.27	-24.20	-24.20
2	60	-0.56	-33.36	-57.56

Once the LID table is established, the cascade diagram is set up with the relevant flowrates of sinks and sources through each interval. The most negative residual value in the cascade diagram indicates the minimum amount of fresh water must be supplied to the process, as can be seen from Figure 4.4 the minimum fresh fiber is 14.95 ton/hr and the minimum waste fiber discharge is 24.95 ton/hr.

Interval	**Load ton/hr** **0.0**	**Interval Load (ΔM_k) ton/hr**	**Sources**	**Source Flow per Interval (ΔW_k), ton/hr**	**Sinks**	**Sink Flow per Interval (ΔG_k), ton/hr**
1	**-8.09**	**-8.09**	**Source 1** **Ψ =-0.27**	**30.07**	**Sink 1** **Ψ^z=-0.2**	**40.0**
2	**-24.20**	−16.12		**59.93**		**45.27**
3	**-43.69**	**-19.49**	**Source 2** **Ψ =-0.56**	**35.05**	**Sink 2** **Ψ=-0.36**	**54.73**
4	**-57.56**	**-13.87**		**24.95**		

Figure 4.3 LID for papermaking example.

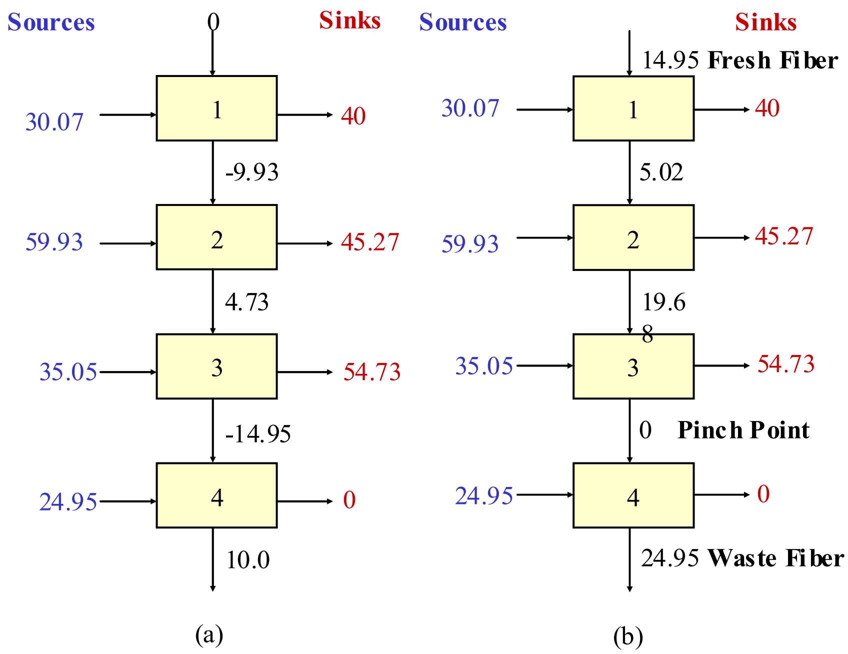


Figure 4.4 Cascade diagram for papermaking example, (a) with infeasibilities (b) revised.

4.5 Conclusions

In this work the systematic algebraic procedure for the targeting of material-recycle networks is extended to property integration. Two case studies were solved to illustrate the applicability of the devised procedure.

4.6 Nomenclature

G Sink (unit) flow, mass or volume/time

M Load, mass or volume/time

$N_{sources}$ Number of process streams (or sources)

N_{sinks} Number of process units (sinks)

W Sink (unit) flow, mass or volume/time

y Contaminant composition of process streams (or sources)

z Allowable contaminant composition of process unit (or sink)

$\bar{k}$ Total number of intervals

Superscripts

min Unit (sink) lower bound of allowable contaminant concentration

max Unit (sink) upper bound of allowable contaminant concentration

Subscripts

i Index for sources

j Index for sinks

k Interval index

Greek Letters

δ Interval Residual, mass or volume/time

Δ Difference between two consecutive intervals

ψ Property operator.

Ψ Adjusted property operator.

CHAPTER V

ALGEBRAIC TARGETING FOR MULTIPLE FRESH RESOURCES

5.1 Literature Review

The process industries are characterized by the significant consumption of fresh resources. One approach towards more sustainable operation is resource conservation through material recycle or reuse. An effective reuse strategy must consider the process as a whole and develop plant-wide strategies. Consequently, process integration has played a major role in developing holistic reuse techniques that emphasize the unity of the process and relate the various sources and users of fresh resources. In particular, mass integration methodology has been developed as a holistic approach to the effective utilization, allocation, transformation, and separation of streams and species.

Recent reviews of mass integration can be found in literature (e.g., Dunn and El-Halwagi, (2003); El-Halwagi and Spriggs, (1998); El-Halwagi, (1997)). In the area of recycle/reuse, much work has been done to target minimum fresh usage and minimum waste discharge for particular material utilities (e.g., water, hydrogen, etc.). Examples of these research efforts can be found in literature (e.g., Manan *et al.*, (2004); Manan and Foo, (2003); El-Halwagi *et al.*, (2003); Hallale, (2002); Alves and Towler, (2002); Polley and Polley, (2000); Dhole *el al.*, (1996); Sorin, M.; Bédard, (1999); Wang and Smith, (1994)).

Notwithstanding the previous work, no graphical or algebraic targeting attempts have been found in the literature that deals with multiple fresh resources targeting.

5.2 Problem Statement

Consider a process with:

- A number ($N_{sources}$) of process streams (or sources) eligible for recycle/reuse. Each source, i, has a flowrate W_i, and composition $y_i, i = 1, 2, \ldots, N_{sources}$.
- A number (N_{sinks}) of process units (sinks). Each sink, j, can accommodate a feed of given flowrate G_j, with z_j^{in} composition that lies within predefined upper and lower bounds $z_j^{\min}$ and $z_j^{\max}$, $j = 1, 2, \ldots, N_{sinks}$.
- F_n Fresh (external) resources with a contaminant concentration of $y_{f_k}, k = 1, 2, \cdots, n$ that can be purchased to supplement the use of process sources in sinks. Each source has a c_k cost per unit mass of fresh associated with it.

The objective is to develop a non-iterative algebraic procedure aimed at minimizing the purchase of fresh resource, maximizing the usage of process sources, and minimizing waste discharge.

5.3 Problem Formulation Background

El-Halwagi et al. (2003) derived the optimality conditions via dynamic programming for single fresh source. They concluded that whenever a fresh source is used to satisfy a sink flow requirement, that sink constitute a local pinch point as show in Figure 5.1.

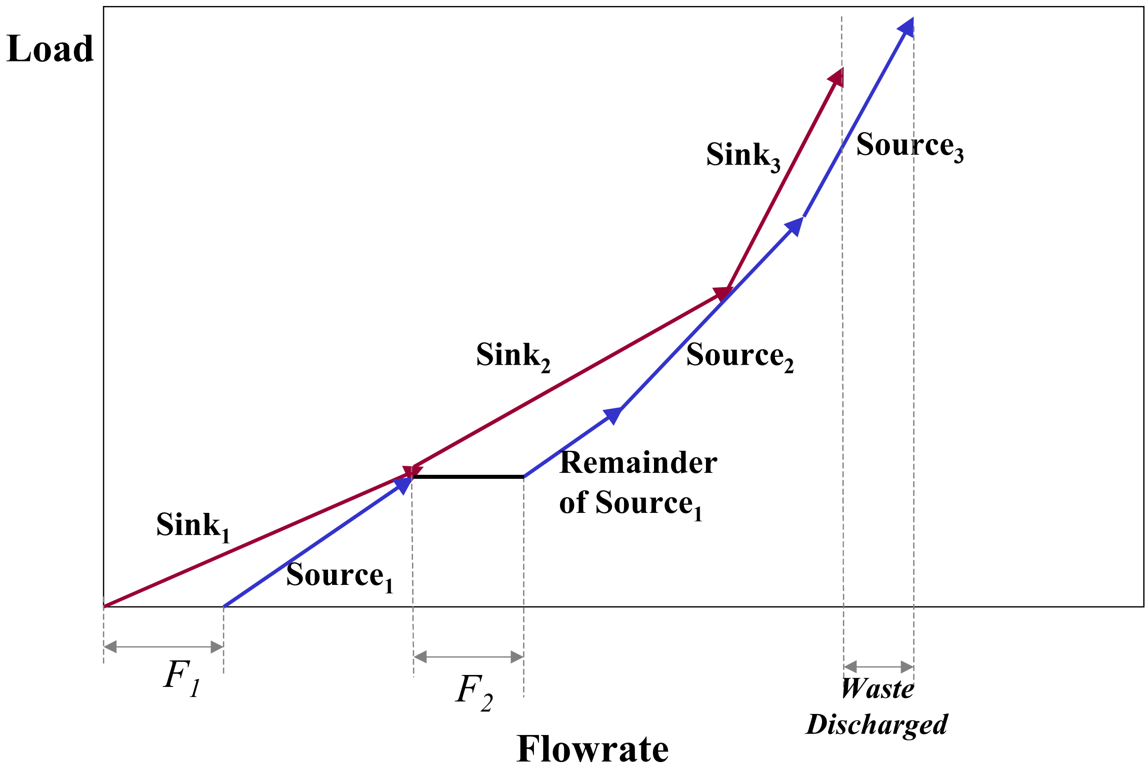


Figure 5.1 Load versus flowrate graph for three sources and three sinks (El-Halwagi *et al* 2003).

Similarly, the optimality conditions would be the same for multiple fresh resources. Provided, there is no flow limitation on fresh resources, the outcome is shown in Figure 5.2.

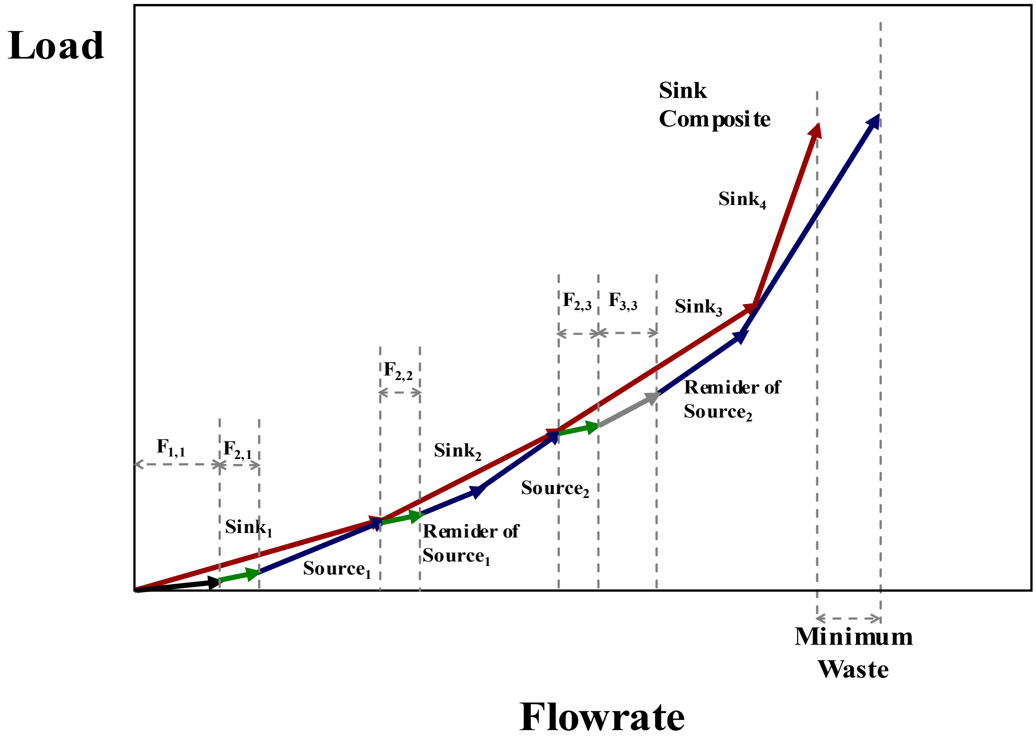


Figure 5.2 Load versus flowrate for multiple fresh resources.

5.4 Derivation of Algebraic Conditions for Optimality

Maximum Fresh Sources per Sink. First let us scrutinize the maximum number of fresh resources per sink. Suppose the following conditions apply for a sink

$$y_{f_1} < z < y_{f_2} < y_{f_3} \tag{5.1}$$

and

$$c_1 > c_2 > c_3 \tag{5.2}$$

This situation is depicted in Figure 5.3. First let us consider F_1 and F_2 as a viable combination to satisfy the flow requirement for the sink. Material balance around the sink j, given that the sink will constitute a local pinch point, is as follows

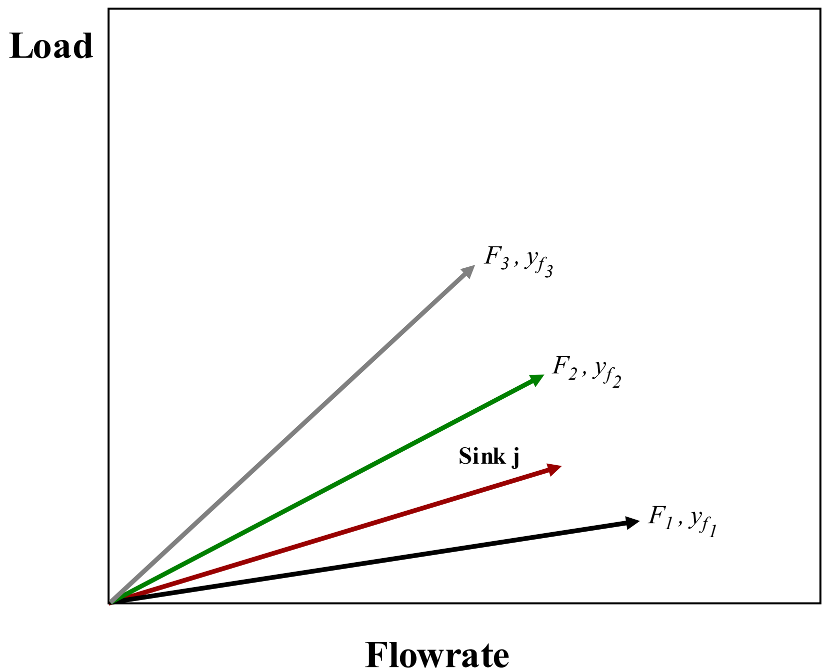


Figure 5.3 Maximum number of fresh resources per sink.

$$G_j = F_1 + F_2 \tag{5.3}$$

Rearranging Equation (5.3) gives

$$F_2 = G_j - F_1 \tag{5.4}$$

Load balance around the sink produces

$$G_j z_j^{\max} = F_1 y_{f_1} + F_2 y_{f_2} \tag{5.5}$$

Substituting Equation (5.4) into Equation (5.5) and rearranging for F_1 yields

$$F_1 = G_j \left(\frac{y_{f_2} - z_j^{\max}}{y_{f_2} - y_{f_1}} \right) \tag{5.6}$$

and

$$F_2 = G_j \left(\frac{z_j^{\max} - y_{f_1}}{y_{f_2} - y_{f_1}} \right) \tag{5.7}$$

$$\text{Cost I } = c_1 F_1 + c_2 F_2 \tag{5.8}$$

Substituting for F_1 and F_2 into cost equation

$$\text{Cost I} = G_j \left[c_1 \left(\frac{y_{f_2} - z_j^{\max}}{y_{f_2} - y_{f_1}} \right) + c_2 \left(\frac{z_j^{\max} - y_{f_1}}{y_{f_2} - y_{f_1}} \right) \right] \tag{5.9}$$

Now let us consider three external resources for the same sink

$$G_j = \overline{F}_1 + \overline{F}_2 + \overline{F}_3 \tag{5.10}$$

Rearranging Equation (5.10) gives

$$\overline{F}_2 = G_j - \overline{F}_1 - \overline{F}_3 \tag{5.11}$$

Load balance around the sink produces

$$G_j z_j^{\max} = \overline{F}_1 y_{f_1} + \overline{F}_2 y_{f_2} + \overline{F}_3 y_{f_3} \tag{5.12}$$

Substituting Equation (5.11) into Equation (5.12)

$$G_j z_j^{\max} = \overline{F}_1 y_{f_1} + \left(G_j - \overline{F}_1 - \overline{F}_3 \right) y_{f_2} + \overline{F}_3 y_{f_3} \tag{5.13}$$

Rearranging Equation (5.13) and solving for $\overline{F}_1$

$$\overline{F}_1 = G_j \frac{y_{f_2} - z_j^{\max}}{y_{f_2} - y_{f_1}} + \overline{F}_3 \frac{y_{f_3} - y_{f_2}}{y_{f_2} - y_{f_1}} \tag{5.14}$$

and

$$\overline{F}_2 = G_j \frac{z_j^{\max} - y_{f_1}}{y_{f_2} - y_{f_1}} - \overline{F}_3 \frac{y_{f_3} - y_{f_1}}{y_{f_2} - y_{f_1}} \tag{5.15}$$

$$\text{Cost II } = c_1 \overline{F}_1 + c_2 \overline{F}_2 + c_3 \overline{F}_3 \tag{5.16}$$

Substituting for $\overline{F}_1$ and $\overline{F}_2$ into cost equation

$$\text{Cost II } = c_1 \overline{F}_1 + c_2 \overline{F}_2 + c_3 \overline{F}_3 \tag{5.17}$$

$$\text{Cost II} = c_1\left(G_j \frac{y_{f_2} - z_j^{\max}}{y_{f_2} - y_{f_1}} + \overline{F}_3 \frac{y_{f_3} - y_{f_2}}{y_{f_2} - y_{f_1}} \right) + c_2\left(G_j \frac{z_j^{\max} - y_{f_1}}{y_{f_2} - y_{f_1}} - \overline{F}_3 \frac{y_{f_3} - y_{f_1}}{y_{f_2} - y_{f_1}} \right) + c_3 \overline{F}_3 \tag{5.18}$$

Rearranging Equation (5.18) gives

$$\text{Cost II} = G_j\left(c_1 \frac{y_{f_2} - z_j^{\max}}{y_{f_2} - y_{f_1}} + c_2 \frac{z_j^{\max} - y_{f_1}}{y_{f_2} - y_{f_1}} \right) + \overline{F}_3\left(c_1 \frac{y_{f_3} - y_{f_2}}{y_{f_2} - y_{f_1}} - c_2 \frac{y_{f_3} - y_{f_1}}{y_{f_2} - y_{f_1}} + c_3 \right) \tag{5.19}$$

$$\text{Cost II-Cost I} = \overline{F}_3\left(c_1 \frac{y_{f_3} - y_{f_2}}{y_{f_2} - y_{f_1}} - c_2 \frac{y_{f_3} - y_{f_1}}{y_{f_2} - y_{f_1}} + c_3 \right) \tag{5.20}$$

Therefore, maximum of two fresh sources dictate that

$$c_3 \geq c_2 \frac{y_{f_3} - y_{f_1}}{y_{f_2} - y_{f_1}} - c_1 \frac{y_{f_3} - y_{f_2}}{y_{f_2} - y_{f_1}} \tag{5.21}$$

or

$$\frac{c_1 - c_3}{y_{f_3} - y_{f_1}} \geq \frac{c_1 - c_2}{y_{f_2} - y_{f_1}} \tag{5.22}$$

One can determine the breaking price of $\overline{F}_3$ above or below which maximum of only two fresh sources exist

$$c_3^* = c_1 - \left(c_1 - c_2\right) \frac{y_{f_3} - y_{f_1}}{y_{f_2} - y_{f_1}} \tag{5.23}$$

However, two fresh resources would be sufficient economically at c_3^*. Therefore, two fresh resources will be considered in the foregoing treatment of the problem.

Criterion I: Single Source below Sink and Multiple Sources above It. Suppose the following conditions apply for a sink as shown in Figure 5.3.

$$y_{f_1} < z < y_{f_2} < y_{f_3} \tag{5.24}$$

and

$$c_1 > c_2 > c_3 \tag{5.25}$$

First let us consider F_1 and F_2. Material balance around the sink j, given that the sink will constitute a local pinch point, is as follows

$$G_j = F_{1,2} + F_2 \tag{5.26}$$

Rearranging Equation (5.26) gives

$$F_2 = G_j - F_{1,2} \tag{5.27}$$

Load balance around the sink produces

$$G_j z_j^{\max} = F_{1,2} y_{f_1} + F_2 y_{f_2} \tag{5.28}$$

Substituting Equation (5.27) into Equation (5.28) and rearranging for $F_{1,2}$ yields

$$F_{1,2} = G_j \left(\frac{y_{f_2} - z_j^{\max}}{y_{f_2} - y_{f_1}} \right) \tag{5.29}$$

and

$$F_2 = G_j \left(\frac{z_j^{\max} - y_{f_1}}{y_{f_2} - y_{f_1}} \right) \tag{5.30}$$

$$\text{Cost I} = c_1 F_{1,2} + c_2 F_2 \tag{5.31}$$

Substituting for $F_{1,2}$ and F_2 into cost equation

$$\text{Cost I} = G_j \left[c_1 \left(\frac{y_{f_2} - z_j^{\max}}{y_{f_2} - y_{f_1}} \right) + c_2 \left(\frac{z_j^{\max} - y_{f_1}}{y_{f_2} - y_{f_1}} \right) \right] \tag{5.32}$$

Similarly for the combination of F_1 and F_3

$$F_{1,3} = G_j \left(\frac{y_{f_3} - z_j^{\max}}{y_{f_3} - y_{f_1}} \right) \tag{5.33}$$

and

$$F_3 = G_j\left(\frac{z_j^{\max} - y_{f_1}}{y_{f_3} - y_{f_1}}\right) \tag{5.34}$$

$$\text{Cost II } = c_1 F_{1,3} + c_3 F_3 \tag{5.35}$$

Substituting for $F_{1,3}$ and F_3 into cost equation

$$\text{Cost II} = G_j\left[c_1\left(\frac{y_{f_3} - z_j^{\max}}{y_{f_3} - y_{f_1}}\right) + c_3\left(\frac{z_j^{\max} - y_{f_1}}{y_{f_3} - y_{f_1}}\right)\right] \tag{5.36}$$

$$\text{Cost I-Cost II} \propto c_1\left[\left(\frac{y_{f_2} - z_j^{\max}}{y_{f_2} - y_{f_1}}\right) - \left(\frac{y_{f_3} - z_j^{\max}}{y_{f_3} - y_{f_1}}\right)\right] + c_2\left(\frac{z_j^{\max} - y_{f_1}}{y_{f_2} - y_{f_1}}\right) - c_3\left(\frac{z_j^{\max} - y_{f_1}}{y_{f_3} - y_{f_1}}\right) \tag{5.37}$$

The first term on the RHS can be simplified as follows

$$\begin{aligned} &c_1\left[\left(\frac{y_{f_2} - z_j^{\max}}{y_{f_2} - y_{f_1}}\right) - \left(\frac{y_{f_3} - z_j^{\max}}{y_{f_3} - y_{f_1}}\right)\right] = \\ &c_1\left[\left(\frac{\left(y_{f_2} - y_{f_1}\right) + \left(y_{f_1} - z_j^{\max}\right)}{y_{f_2} - y_{f_1}}\right) - \left(\frac{\left(y_{f_3} - y_{f_1}\right) + \left(y_{f_1} - z_j^{\max}\right)}{y_{f_3} - y_{f_1}}\right)\right] \end{aligned} \tag{5.38}$$

$$\begin{aligned} c_1\left[\left(\frac{y_{f_2} - z_j^{\max}}{y_{f_2} - y_{f_1}}\right) - \left(\frac{y_{f_3} - z_j^{\max}}{y_{f_3} - y_{f_1}}\right)\right] &= c_1\left[1 + \frac{\left(y_{f_1} - z_j^{\max}\right)}{\left(y_{f_2} - y_{f_1}\right)} - 1 - \frac{\left(y_{f_1} - z_j^{\max}\right)}{\left(y_{f_3} - y_{f_1}\right)}\right] \\ &= c_1\left[\frac{\left(z_j^{\max} - y_{f_1}\right)}{\left(y_{f_3} - y_{f_1}\right)} - \frac{\left(z_j^{\max} - y_{f_1}\right)}{\left(y_{f_2} - y_{f_1}\right)}\right] \end{aligned} \tag{5.39}$$

Then Equation (5.37) becomes

$$\text{Cost I-Cost II} \propto \frac{c_1}{\left(y_{f_3} - y_{f_1}\right)} - \frac{c_1}{\left(y_{f_2} - y_{f_1}\right)} + \frac{c_2}{\left(y_{f_2} - y_{f_1}\right)} - \frac{c_3}{\left(y_{f_3} - y_{f_1}\right)} \tag{5.40}$$

or

$$\text{Cost I-Cost II} \propto \frac{c_1 - c_3}{\left(y_{f_3} - y_{f_1}\right)} - \frac{c_1 - c_2}{\left(y_{f_2} - y_{f_1}\right)} \tag{5.41}$$

$$\text{Cost I-Cost II} \propto \frac{\Delta c_{1,3}}{\Delta y_{f_{3,1}}} - \frac{\Delta c_{1,2}}{\Delta y_{f_{2,1}}} \tag{5.42}$$

Therefore, if

$\frac{\Delta c_{1,3}}{\Delta y_{f_{3,1}}} > \frac{\Delta c_{1,2}}{\Delta y_{f_{2,1}}}$ use fresh resource combination F_1 and F_2 and visa versa.

Criterion II: Multiple Sources below Sink and a Single Source above It. Figure 5.4 depict a case when single external source below a sink and a couple above it, according to the following criteria

$$y_{f_1} < y_{f_2} < z < y_{f_3} \tag{5.43}$$

and

$$c_1 > c_2 > c_3 \tag{5.44}$$

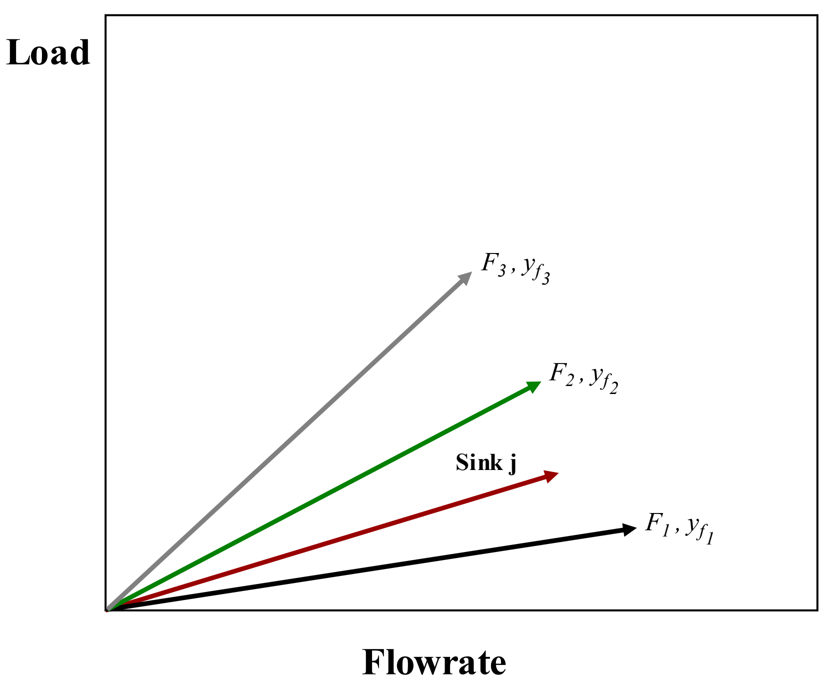


Figure 5.4 Single fresh source below a sink and a couple above it.

Let us examine the combination of F_1 and F_3 as a possible choice. Performing material balance around sink j as follows

$$G_j = F_1 + F_{3,1} \tag{5.45}$$

Rearranging Equation (5.45) gives

$$F_{3,1} = G_j - F_1 \tag{5.46}$$

Load balance around the same sink produces

$$G_j z_j^{\max} = F_1 y_{f_1} + F_{3,1} y_{f_3} \tag{5.47}$$

Substituting Equation (5.46) into Equation (5.47) and rearranging for F_1 yields

$$F_1 = G_j \left(\frac{y_{f_3} - z_j^{\max}}{y_{f_3} - y_{f_1}} \right) \tag{5.48}$$

and

$$F_{3,1} = G_j \left(\frac{z_j^{\max} - y_{f_1}}{y_{f_3} - y_{f_1}} \right) \tag{5.49}$$

$$\text{Cost I} = c_1 F_1 + c_3 F_{3,1} \tag{5.50}$$

Substituting for F_1 and $F_{3,1}$ into cost equation

$$\text{Cost I} = G_j \left[c_1 \left(\frac{y_{f_3} - z_j^{\max}}{y_{f_3} - y_{f_1}} \right) + c_3 \left(\frac{z_j^{\max} - y_{f_1}}{y_{f_3} - y_{f_1}} \right) \right] \tag{5.51}$$

Similarly for the combination of F_2 and F_3 to the same sink yield

$$F_2 = G_j \left(\frac{y_{f_3} - z_j^{\max}}{y_{f_3} - y_{f_2}} \right) \tag{5.52}$$

and

$$F_{3,2} = G_j \left(\frac{z_j^{\max} - y_{f_2}}{y_{f_3} - y_{f_2}} \right) \tag{5.53}$$

$$\text{Cost II } = c_2 F_2 + c_3 F_{3,2} \tag{5.54}$$

Substituting for F_2 and $F_{3,2}$ into cost equation

$$\text{Cost II} = G_j \left[c_2 \left(\frac{y_{f_3} - z_j^{\max}}{y_{f_3} - y_{f_2}} \right) + c_3 \left(\frac{z_j^{\max} - y_{f_2}}{y_{f_3} - y_{f_2}} \right) \right] \tag{5.55}$$

$$\text{Cost I-Cost II} \propto c_3 \left[\left(\frac{z_j^{\max} - y_{f_1}}{y_{f_3} - y_{f_1}} \right) - \left(\frac{z_j^{\max} - y_{f_2}}{y_{f_3} - y_{f_2}} \right) \right] + c_1 \left(\frac{y_{f_3} - z_j^{\max}}{y_{f_3} - y_{f_1}} \right) - c_2 \left(\frac{y_{f_3} - z_j^{\max}}{y_{f_3} - y_{f_2}} \right) \tag{5.56}$$

The first term on the RHS can be simplified as follows

$$\begin{aligned} & c_3 \left[\left(\frac{z_j^{\max} - y_{f_1}}{y_{f_3} - y_{f_1}} \right) - \left(\frac{z_j^{\max} - y_{f_2}}{y_{f_3} - y_{f_2}} \right) \right] = \\ & c_3 \left[\left(\frac{\left(z_j^{\max} - y_{f_3}\right) + \left(y_{f_3} - y_{f_1}\right)}{y_{f_3} - y_{f_1}} \right) - \left(\frac{\left(z_j^{\max} - y_{f_3}\right) + \left(y_{f_3} - y_{f_2}\right)}{y_{f_3} - y_{f_2}} \right) \right] \end{aligned} \tag{5.57}$$

$$\begin{aligned} c_3 \left[\left(\frac{z_j^{\max} - y_{f_1}}{y_{f_3} - y_{f_1}} \right) - \left(\frac{z_j^{\max} - y_{f_2}}{y_{f_3} - y_{f_2}} \right) \right] &= c_3 \left[\frac{\left(z_j^{\max} - y_{f_3}\right)}{\left(y_{f_3} - y_{f_1}\right)} + 1 - \frac{\left(z_j^{\max} - y_{f_3}\right)}{\left(y_{f_3} - y_{f_2}\right)} - 1 \right] \\ &= c_3 \left[\frac{\left(z_j^{\max} - y_{f_3}\right)}{\left(y_{f_3} - y_{f_1}\right)} - \frac{\left(z_j^{\max} - y_{f_3}\right)}{\left(y_{f_3} - y_{f_2}\right)} \right] \end{aligned} \tag{5.58}$$

Then Equation (5.56) becomes

$$\text{Cost I-Cost II} \propto \frac{c_3}{\left(y_{f_3} - y_{f_2}\right)} - \frac{c_3}{\left(y_{f_3} - y_{f_1}\right)} + \frac{c_1}{\left(y_{f_3} - y_{f_1}\right)} - \frac{c_2}{\left(y_{f_3} - y_{f_2}\right)} \tag{5.59}$$

or

$$\text{Cost I-Cost II} \propto \frac{c_1 - c_3}{\left(y_{f_3} - y_{f_1}\right)} - \frac{c_2 - c_3}{\left(y_{f_3} - y_{f_2}\right)} \tag{5.60}$$

$$\text{Cost I-Cost II} \propto \frac{\Delta c_{1,3}}{\Delta y_{f_{3,1}}} - \frac{\Delta c_{2,3}}{\Delta y_{f_{3,2}}} \tag{5.61}$$

Therefore, if

$\frac{\Delta c_{1,3}}{\Delta y_{f_{3,1}}} > \frac{\Delta c_{2,3}}{\Delta y_{f_{3,2}}}$ use fresh resource combination F_2 and F_3 and visa versa.

Criterion III: Fresh Source Coincide with Sink and Single Source below and above That Sink. Suppose the following conditions apply for a sink

$$y_{f_1} < y_{f_2} = z < y_{f_3} \tag{5.62}$$

and

$$c_1 > c_2 > c_3 \tag{5.63}$$

This situation is portrayed in Figure 5.5

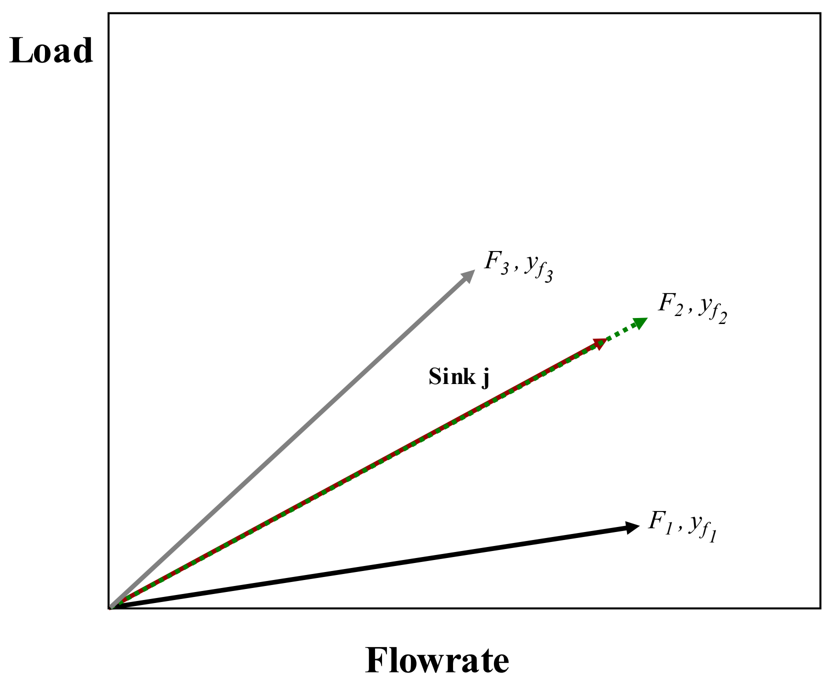


Figure 5.5 Fresh source coincide with sink and a single source above and below it.

Material balance around the sink j, given that the sink will constitute a local pinch point, is as follows

$$G_j = F_2 \tag{5.64}$$

$$\text{Cost I } = c_2 F_2 = c_2 G_j \tag{5.65}$$

Now let us consider a combination of F_1 and F_3. Material balance around the sink j, given that the sink will constitute a local pinch point, is as follows

$$F_{1,3} = G_j\left(\frac{y_{f_3} - z_j^{\max}}{y_{f_3} - y_{f_1}}\right) \tag{5.66}$$

and

$$F_3 = G_j\left(\frac{z_j^{\max} - y_{f_1}}{y_{f_3} - y_{f_1}}\right) \tag{5.67}$$

$$\text{Cost II } = c_1 F_{1,3} + c_3 F_3 \tag{5.68}$$

Substituting for $F_{1,3}$ and F_3 into cost equation

$$\text{Cost II} = G_j\left[c_1\left(\frac{y_{f_3} - z_j^{\max}}{y_{f_3} - y_{f_1}}\right) + c_3\left(\frac{z_j^{\max} - y_{f_1}}{y_{f_3} - y_{f_1}}\right)\right] \tag{5.69}$$

$$\text{Cost I-Cost II} \propto c_2 - \left[c_1\left(\frac{y_{f_3} - z_j^{\max}}{y_{f_3} - y_{f_1}}\right) + c_3\left(\frac{z_j^{\max} - y_{f_1}}{y_{f_3} - y_{f_1}}\right)\right] \tag{5.70}$$

The second term on the RHS can be simplified as follows

$$\left[c_1 - c_1\left(\frac{z_j^{\max} - y_{f_1}}{y_{f_3} - y_{f_1}}\right) + c_3\left(\frac{z_j^{\max} - y_{f_1}}{y_{f_3} - y_{f_1}}\right)\right] \tag{5.71}$$

Then Equation (5.71) becomes

$$\text{Cost I-Cost II} \propto c_2 - \left[c_1 - c_1 \left(\frac{z_j^{\max} - y_{f_1}}{y_{f_3} - y_{f_1}} \right) + c_3 \left(\frac{z_j^{\max} - y_{f_1}}{y_{f_3} - y_{f_1}} \right) \right] \tag{5.72}$$

Then Equation (5.72) becomes

$$\text{Cost I-Cost II} \propto \frac{c_1 - c_3}{\left(y_{f_3} - y_{f_1} \right)} - \frac{c_1 - c_2}{\left(z_j^{\max} - y_{f_1} \right)} \tag{5.73}$$

Therefore, if

$\frac{\Delta c_{1,3}}{\Delta y_{f_{3,1}}} < \frac{\Delta c_{1,2}}{\Delta y_{f_{2,1}}}$ use fresh resource F_2 alone otherwise use a combination of F_1 and F_3.

Criterion IV: Multiple Sources below Sink and No Source above It. Only single fresh source ought to be used to minimize cost. Namely, the lowest source cost.

Criterion V: Multiple Sources above Sink and No Source below It. Might be feasible if and only if process sources are available below sink.

Process Sources Prioritization Rule. A systematic methodology for mixing process sources to satisfy the flow and load requirement of a sink is derived as follows. Figure 5.6 represents a process such that

$y_1 < z_j^{\max} < y_2 < y_3$.

The goal is to minimize the usage of process sources below the specified sink in order to conserve its use for the following more demanding sink in line. If process sources 1 and 2 are mixed then

$$G_j = \alpha_1 w_1 + \alpha_2 w_2 \tag{5.74}$$

Rearranging Equation (5.74) gives

$$\alpha_2 w_2 = G_j + \alpha_1 w_1 \tag{5.75}$$

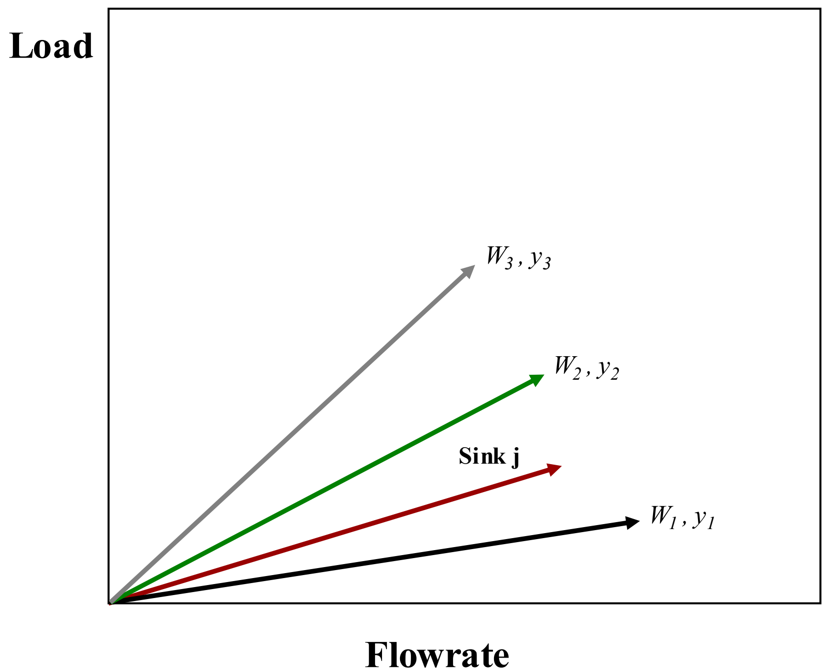


Figure 5.6 Process sources prioritization rule.

Load balance around the same sink produces

$$G_j z_j^{\max} = \alpha_1 w_1 y_1 + \alpha_2 w_2 y_2 \tag{5.76}$$

Substituting Equation (5.75) into Equation (5.76) and rearranging for $\alpha_1 w_1$ yields

$$\alpha_1 w_1 = G_j \left(\frac{y_2 - z_j^{\max}}{y_2 - y_1} \right) \tag{5.77}$$

Similarly for mixing process sources 1 and 3, one can get

$$\beta_1 w_1 = G_j \left(\frac{y_3 - z_j^{\max}}{y_3 - y_1} \right) \tag{5.78}$$

Subtracting Equation (5.78) from Equation (5.77) yield

$$\alpha_1 - \beta_1 \propto \left(\frac{y_2 - z_j^{\max}}{y_2 - y_1} \right) - \left(\frac{y_3 - z_j^{\max}}{y_3 - y_1} \right) \tag{5.79}$$

Simplifying Equation (5.79) gives

$$\alpha_1 - \beta_1 \propto 1 - \frac{z_j^{\max} - y_1}{y_2 - y_1} - 1 + \frac{z_j^{\max} - y_1}{y_3 - y_1} \tag{5.80}$$

or

$$\alpha_1 - \beta_1 \propto \frac{1}{y_3 - y_1} - \frac{1}{y_2 - y_1} \tag{5.81}$$

The right hand side of Equation (5.81) is always negative. Therefore, flow optimality requires the exploitation of the second process source prior to considering the third process source.

It is worth mentioning that process sources have a zero cost associated with them. To this end we are in a position to proceed to solve a case study.

5.5 Case Study

The pertinent sinks and sources information regarding this case study is shown in Table 5.1, the specifications of the fresh resources available in the market are given in Table 5.2.

The first step is determining the most economical combination of fresh sources for each sink ahead of the targeting procedure without considering the interaction of process sources. Applying Equation (5.42) to the first sink produces

$$c(F_1 + F_2) - c(F_1 + F_3) \propto 31.6 - 40 \cong -ve$$

Therefore, the most favored fresh resource combination is the first two sources. The second sink belongs to the third criterion where one fresh coincide with the sink, applying Equation (5.73) yield

$$c(F_2) - c(F_1 + F_3) \propto 31.6 - 40 \cong -ve$$

Table 5.1 Sources and sinks information for example 1.

Sink	**Flowrate, ton/hr**	z^{max}
G_1	100	0.1
G_2	20	0.15
G_3	60	0.2
Sources	**Flowrate, ton/hr**	y
W_1	20	0.12
W_2	70	0.2
W_3	100	0.25

Table 5.2 Fresh resources specifications for example 1.

Fresh Source	y_f	**Cost, $/ton**
F_1	0.05	7
F_2	0.15	3
F_3	0.24	1

This indicates that the second fresh source would be the only consideration once the targeting phase commences. Criterion III govern the most economical usage for the third sink, Equation (5.60) is applied to the sink giving

$$c(F_1+F_3)-c(F_2+F_3)\propto 31.6-22.2\cong +ve$$

The result signifies the usage of combination of the second and third fresh sources.

Forward Targeting. Let us begin the targeting procedure by starting with the most stringent sink and moving to the next and so forth. Table 5.3 shows the sources above the first sink and their reduced cost when combined with the first fresh source, using the first criterion the order at which the combination showed follow is W_1, W_2, and then F_2.

Making a flow and load balance around the first sink by considering the first two process sources only would indicate that mixing 56 ton/hr of fresh source 1 with 20 ton/hr of process source 1, and 24 ton/hr of process source 2 meets the sink requirement. The reminder of process source 2, 46 ton/hr, is available for the following sinks.

Based on the analysis done earlier for the allocation of fresh sources to respective sinks, Fresh source 2 is the only available option for the second sink. Therefore, a flow of 20 ton/hr of fresh source 2 ought to be supplemented to the sink.

Table 5.3 Forward targeting source prioritization for the first sink.

Source	**Flow, ton/hr**	**y**	**Cost, $/ton**	$\frac{c_1 - c_i}{\left(y_i - y_{f_1}\right)}$
W_1	20	0.12	0.0	100.0
F_2	-	0.15	3.0	40.0
W_2	70	0.20	0.0	46.7
W_3	100	0.25	0.0	35.0

Moving on to the third sink, using Table 5.4 and applying the second criterion we are able to prioritize the usage of sources in order to fulfill the sink requirement. The order at which sources are utilized along with F_2 is W_3, then F_3.

Flow and load balance around the third sink reveals the need for only 7 ton/hr of fresh source 2. The total cost of supplementing fresh sources to the process is:

Total Cost = (56)(7) + (27)(3) = \$473/hr

Table 5.4 Forward targeting source prioritization for the third sink.

Source	Flow, ton/hr	y	Cost, $/ton	$\frac{c_2 - c_i}{\left(y_i - y_{f_2}\right)}$
F_3	-	0.24	1.00	22.2
W_3	100	0.25	0.00	30.0

This value is higher than that obtained ($466/hr) using LINGO optimization software.

Backward Targeting. A different outcome is obtained if we start the targeting from the most relaxed sink. Starting with the third sink, source prioritization rule dictates exploiting the second process source, as it has the same contaminant concentration of the sink, prior to considering any other source.

Since $W_2 > G_2$, third sink is totally satisfied in terms of flow and load by the second source. The reminder of process source 2 to be available for reuse to other sinks is

$W_2^{'} = W_2 - G_2 = 70 - 60 = 10$ ton/hr

As for the second sink, source prioritization is applied again by mixing the first and second process sources to fulfill the flow requirement of the sink. Simple mass balance reveals that 7.5 ton/hr of $W_2^{'}$ and 12.5 ton/hr of W_1 is sufficient for sink 2. The reminder of used sources is as follows

$W_2^{''} = 10 - 7.5 = 2.5$ ton/hr , and

$W_1^{'} = 20 - 12.5 = 7.5$ ton/hr

Finally, source prioritization for mixing sources with the first fresh source to the first sink is given in Table 5.5.

The most economical order at which sources are blended is $\boldsymbol{W_1}'$, $\boldsymbol{W_2}''$, and then F_2. The outcome of the mass balance on the sink gives:

$F_1 = 49$ ton/hr , and

$F_2 = 41$ ton/hr

The total cost for the recycle/reuse problem is:

Total Cost = (49)(7) + (41)(3) = \$466/hr

This value conform to the solution obtained using LINGO

Table 5.5 Backward targeting source prioritization for the first sink.

Source	**Flow, ton/hr**	**y**	**Cost, \$/ton**	$\frac{c_1 - c_i}{\left(y_i - y_{f_1}\right)}$
$\boldsymbol{W_1}'$	12.5	0.12	0.0	100.0
$\boldsymbol{F_2}$	-	0.15	3.0	40.0
$\boldsymbol{W_2}''$	2.5	0.20	0.0	46.7
$\boldsymbol{W_3}$	100	0.25	0.0	35.0

Even though backward targeting produces accurate results, it can be rebuttal easily by considering Figure 5.7. In this case $c_1 \gg c_2$, therefore if backward targeting is adopted most if not all of the process source will be allocated to the second sink resulting in enduring higher cost of fresh resource supply.

5.6 Conclusions

In this work the importance of process integration for the whole process as a single entity is stressed again. Looking at the process unit by unit is misleading and could lead to higher targets than the minimum one.

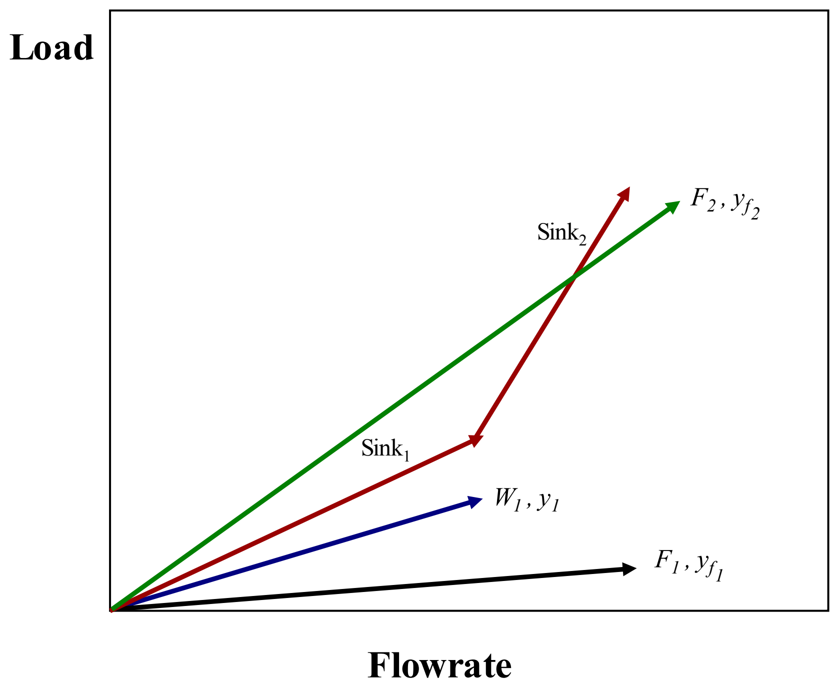


Figure 5.7 Rebuttal to backward targeting.

5.7 Nomenclature

G Sink (unit) flow, mass or volume/time

M Load, mass or volume/time

$N_{sources}$ Number of process streams (or sources)

N_{sinks} Number of process units (sinks)

W Sink (unit) flow, mass or volume/time

y Contaminant composition of process streams (or sources)

z Allowable contaminant composition of process unit (or sink)

Superscripts

min Unit (sink) lower bound of allowable contaminant concentration

max Unit (sink) upper bound of allowable contaminant concentration

Subscripts

i Index for sources

j Index for sinks

CHAPTER VI

A MATHEMATICAL PROGRAMMING APPROACH TO MATERIAL REUSE AND INTERCEPTION NETWORKS

6.1 Literature Review

The previous chapters have presented systematic methods to the targeting of material reuse using algebraic techniques. In spite of the usefulness of these algebraic techniques, they have the following tow main limitations:

- Difficulty in handling multiple fresh streams in conjunction with process streams
- Inability to systematically make optimum decisions on intercepting the process sources to minimize the cost of the system

In response to these limitations, this chapter presents a mathematical programming approach that seeks to address the aforementioned problems. Mathematical programming techniques have also been proposed in literature to solve the recycle/reuse problems (e.g., Savelski and Bagajewicz, 2001, 2001) including multicomponent systems (e.g., Alva-Argaez et. al., 1999; Benko et. al., 2000 and Dunn et. al., 2001). Additionally, similar methods have been developed for unsteady-state and batch systems (e.g., Wang and Smith, 1995, Almato et. al., 1997, and Zhou et al., 2001).

In some cases, direct recycle alone is not sufficient to reach the desired target of fresh usage and waste discharge. This limitation is caused by excessive content of impurities in the process sources such that the recycle opportunities are limited. In such cases, it is necessary to use interception devices. Interception implies the use of a separation unit or network to remove targeted species (e.g., impurities) from in-plant streams. El-Halwagi et al. (1996) introduced the concept of synthesizing waste interception networks and applied it to the use of mass-separating agents to separate impurities from process sources prior to recycle. Gabriel and El-Halwagi (2005) proposed an optimization-based approach to the simultaneous interception and recycle of streams. They used problem reformulation to insure global solution. Gabriel and El-Halwagi used two main assumptions in problem reformulation:

1. A single fresh sources is available for service
2. The cost of intercepting a process source is proportional to the load removed from the stream.

In the following, the two assumptions will be relaxed and a new formulation will be presented.

6.2 Problem Statement

The following problem statement is a generalized version of the one proposed by Gabriel and El-Halwagi (2005). It can be stated as follows:

Given a process with:

- A set of process sinks (units): $\text{SINKS} = \{j \mid j = 1, \cdots, N_{sinnks}\}$. Each sinks requires a given flowrate, G_j, and a given composition, z_j^{in}, that satisfies the following constraint:

  $$z_j^{\min} \le \mathrm{z_j^{in}} \le z_j^{\max} \qquad \forall j \in \{1, \cdots, N_{sinks}\} \tag{6.1}$$

  where $z_j^{\min}$ and $z_j^{\max}$ are given lower and upper bounds on acceptable compositions to unit j.

- A set of process sources: $\text{SOURCES} = \{i \mid i = 1, \cdots, N_{sources}\}$ which can be recycled/reused in process sinks? Each sources has a given flowrate, F_i, and a given composition, y_i^{in}.
- A set of fresh sources: FRESH = $\{f \mid f = 1,2, \ldots, N_{Fresh}\}$. Each fresh source has a given cost, C_f, expressed as \$/kg of the fresh , and a given composition, y_i^{in}. The flowrate of each rich stream, F_i, is unknown and is to be determined through optimization.
- A set of interception units: $\text{INTERCEPTORS} = \{k \mid k = 1, \cdots, N_{\text{int}}\}$ that can be used to remove the targeted species from the sources.

The goal is to develop an optimization formulation whose objective is to minimize the total cost of the fresh sources and interception. This formulation will provide answers to the following design questions:

1. How should the sources be allocated to sinks?
2. Should a source be intercepted? To what extent? Where the intercepted source should be allocated?
3. Should sources be segregated or mixed? How?
4. Which fresh sources should be used? What are their optimal flowrates?
5. How much waste should be discharged?

6.3 Problem Representation

A source-interception-sink representation will be used. This representation is an extension of the one proposed by Gabriel and El-Halwagi (2005) with the key difference being the use of multiple fresh sources. This representation is shown in Figure 6.1. Each segregated process source is split into several fractions. The flowrate of each split is unknown and will be determined through optimization. Each split is fed to the interception network where its composition may be altered. The cost of interception is a function of the flowrate of the stream and the extent of interception. If no interception is performed on the source, the interception cost is zero and the stream passes unchanged through the interception network. The streams leaving the interception network are allowed to mix and fed to the process sinks. The extent of mixing is unknown and is to be determined as part of solving the optimization problem. Sources that are not assigned to process sinks are allocated to waste.

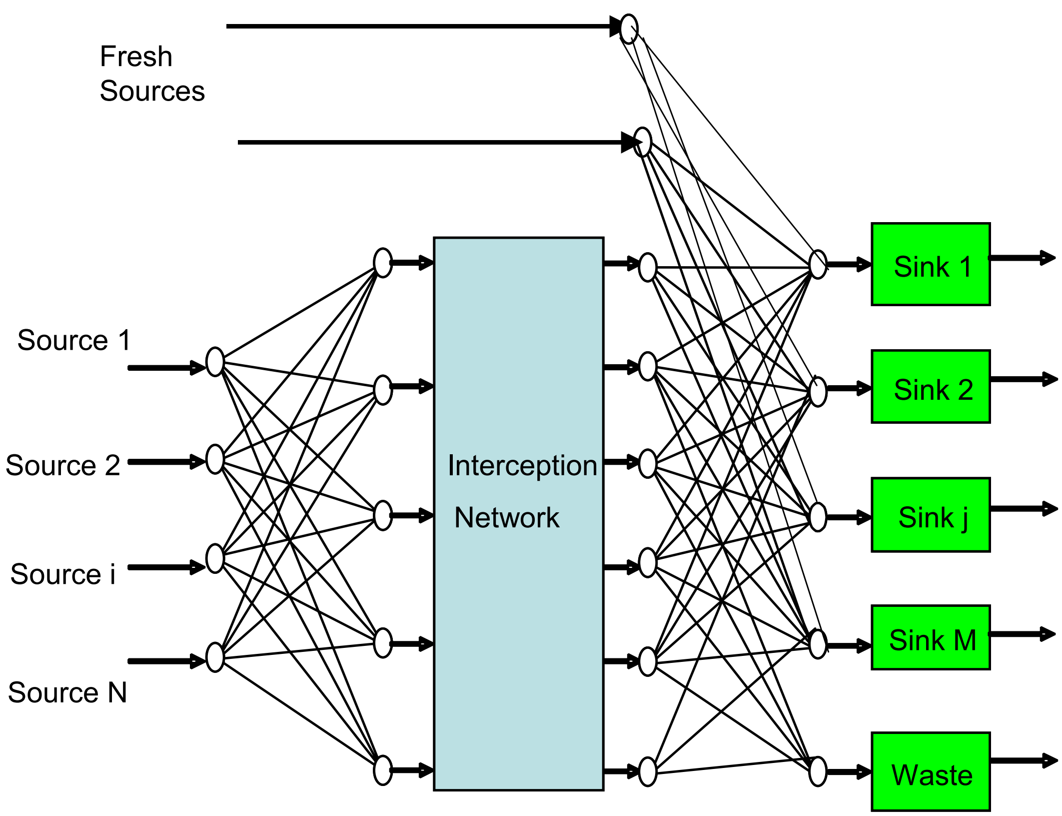


Figure 6.1 Structural representation of the problem.

6.4 Optimization Formulation

The general formulation to solve the problem is a mixed-integer nonlinear program (MINLP) as shown by Gabriel and El-Halwagi (2005).The global solution of such an MINLP is typically an elusive task. Therefore, it is useful to reformulate the problem to make it globally solvable using commercial optimization software. Therefore, we adopt the following assumptions:

1. No mixing of sources is allowed before interception; mixing is used primarily after interception and before entering the sinks.
2. Each interceptor is discretized into a number of interceptors with given removal efficiencies (see Figure 6.2).
3. Cost of each discretized interceptor with a given removal efficiency is evaluated as a convex function of flowrate, $f_u(w_u)$, where w_u is the flowrate passing through the uth interceptor.

We are now in a position to express the reformulated mathematical formulation. It will be described for one fresh source but can be easily described for multiple fresh streams.

Objective Function:

Minimize total annualized cost =

$$C_{Fresh} \cdot \sum_{j=1}^{N_{Sinks}} Fresh_j + \sum_u f_u(w_u) + C_{waste} \cdot waste \tag{6.2}$$

where all the flowrates are given on an annual basis, C_{Fresh} is the cost of the fresh resource ($/amount of resource), $Fresh_j$ is the amount of fresh resource fed to the j^{th} sink (mass per year), $f_u(w_u)$ is the convex cost function of interceptor u, w_u is the flowrate passing through the u^{th} interceptor, C_{waste} is the annual waste treatment cost and *waste* is the total amount of flow going to waste (tons/yr). The constraints of the program are

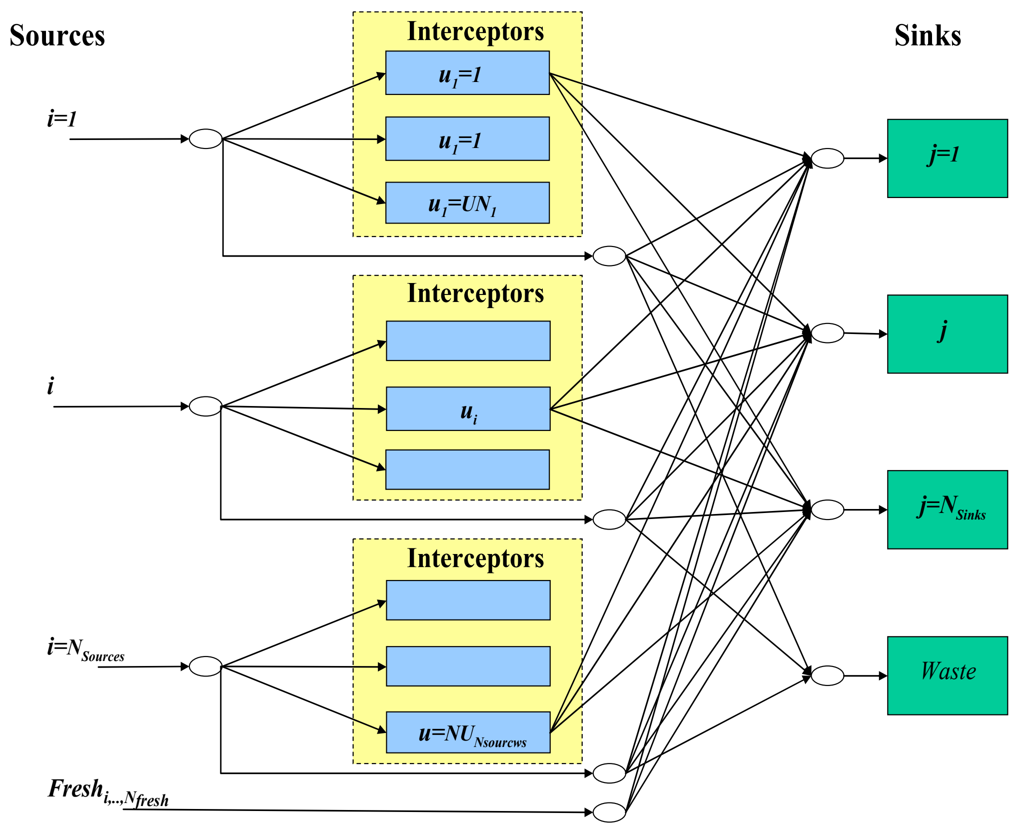


Figure 6.2 Structural representation of the reformulated problem.

similar to the ones described by Gabriel and El-Halwagi (2005). The key difference with the work of Gabriel and El-Halwagi is that instead of a simple cost function of interceptor which is proportional to the load removed by the interceptor, we introduce a convex cost function which is dependent of the flowrate of the feed to the interceptor. This program can be solved globally using commercial optimization software LINGO.

6.5 Case Study

To illustrate the applicability of the new methodology, we address the problem posed by Gabriel and El-Halwagi (2005). This is a water recycle/reuse case study with three process sources and two process sinks. Three interception technologies are considered. The interception costs were reformulated from the original case study to be described in terms of flowrate (instead of load removed). Table 6.1 summarizes the data for the sources and the sinks. Table 6.2 summarizes the data for the fresh sources. The cost of fresh water is assigned to be \$0.13/ton and the waste treatment cost is \$0.22/ton of effluent. A basis of 8,000 operating hours per year is selected. Cost data for each technology operating at various pollutant-removal efficiencies on each source are assigned in Table 6.3 through Table 6.5. The objective of the case study is to minimize the total cost of the system (including fresh usage, interception, and waste treatment) while satisfying all the process demands.

Following the developed reformulation approach, an LP was developed. The LP was then solved using the software LINGO. The minimum total annualized cost was found to be \$54,420/year. No fresh is needed while 30 tons/hr of effluent are fed to wastewater treatment. A portion of source 3 (53 tons/hr) is intercepted using a stream stripper with 10% removal efficiency. The system configuration is illustrated in Fig. 4. These results are consistent with the solution found by Gabriel and El-Halwagi (2005).

Table 6.1 Process information for case study (Gabriel and El-Halwagi, 2005).

Sinks	**Flow, ton/hr**	**Maximum Inlet Concentration, ppm**	**Load, kg/hr**
1	200	20	4
2	80	75	6
Sources	**Flow, ton/hr**	**Concentration, ppm**	**Load, kg/hr**
1	150	10	1.5
2	60	50	3
3	100	85	8.5

Table 6.2 Fresh sources cost data.

Fresh Sources	**Concentration, ppm**	**Cost, $/ton**
1	0	0.13
2	15	0.97
3	25	0.89

Table 6.3 Cost for each technology operating at different contaminant-removal efficiencies for source 1.

Technology	**Removal Efficiency, %**	**Cost, $/kg waste**
Stripping	10	0.68
	20	1.66
	30	3.06
	40	5.00
	50	7.30
	60	9.84
	70	13.16
	80	17.92
	90	26.64
Ion Exchange	10	0.81
	20	1.98
	30	3.66
	40	5.96
	50	8.75
	60	11.76
	70	15.75
	80	21.44
	90	31.95
Adsorption	10	0.88
	20	2.14
	30	3.99
	40	6.48
	50	9.45
	60	12.78
	70	17.08
	80	23.28
	90	34.56

Table 6.4 Cost for each technology operating at different contaminant-removal efficiencies for source 2.

Technology	**Removal Efficiency, %**	**Cost, $/kg waste**
Stripping	10	2.70
	20	6.60
	30	12.30
	40	20.00
	50	29.00
	60	39.30
	70	52.50
	80	71.60
	90	106.20
Ion Exchange	10	3.25
	20	7.90
	30	14.70
	40	24.00
	50	35.00
	60	47.10
	70	63.00
	80	86.00
	90	127.80
Adsorption	10	3.50
	20	8.60
	30	15.90
	40	25.80
	50	37.75
	60	51.00
	70	68.25
	80	92.80
	90	138.15

Table 6.5 Cost for each technology operating at different contaminant-removal efficiencies for source 3.

Technology	Removal Efficiency, %	Cost, $/kg waste
Stripping	10	3.83
	20	9.35
	30	17.34
	40	28.22
	50	41.23
	60	55.59
	70	74.38
	80	101.32
	90	150.71
Ion Exchange	10	4.59
	20	11.22
	30	20.91
	40	34.00
	50	49.30
	60	66.81
	70	89.25
	80	121.72
	90	180.54
Adsorption	10	5.02
	20	12.24
	30	22.44
	40	36.72
	50	53.55
	60	72.42
	70	96.99
	80	131.92
	90	195.84

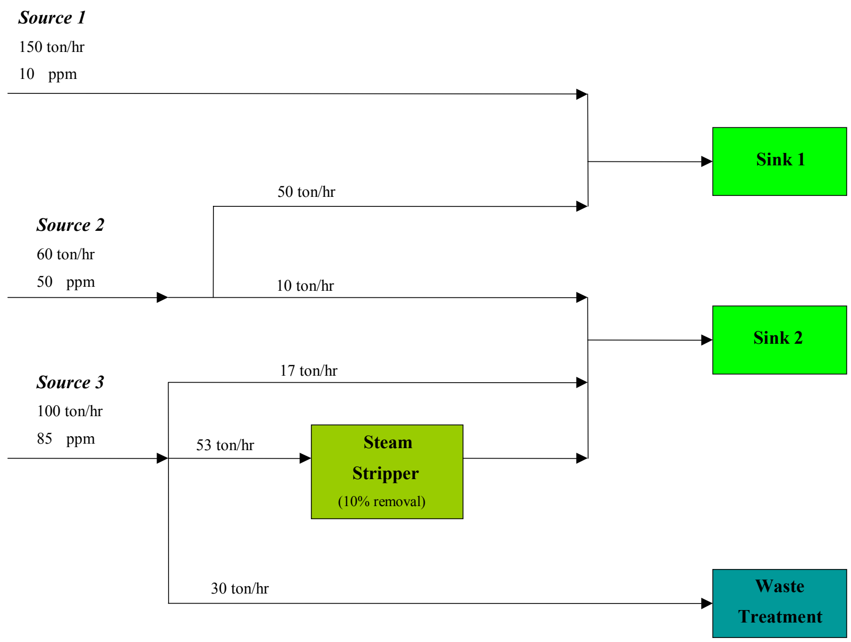


Figure 6.3 Optimal solution to case study.

6.6 Conclusion

In this work, we have addressed the problem of simultaneously synthesizing waste interception and recycle/reuse network. Using convexification, the problem was reformulated to enable global solution of the optimization formulation using commercial software. In particular, a convex cost function was used for interception as a function of flowrate. A case study was solved to illustrate the validity of the developed formulation.

CHAPTER VII

CONCLUSIONS AND RECOMMENDATIONS

This dissertation has introduced several algebraic procedures to the targeting of material recycle networks. The addressed problems involved the allocation of process streams and fresh sources to process units (sinks) with the objective of minimizing fresh purchase and waste discharge. Composition- and property-based constraints were addressed. Several systematic non-iterative algebraic approaches were developed to identify rigorous targets for minimum usage of fresh resources, maximum recycle of process resources and minimum discharge of waste. These targets were identified a priori and without commitment to the detailed design of the recycle/reuse network. The approach is valid for both pure and impure fresh resources. It was also shown that for the general recycle problem, neither the forward solution nor the backward targeting approach is guaranteed to provide the global solution. Instead, the system should be treated in an integrated manner as a whole. Finally, for more complex cases with multiple fresh sources and with interception networks, a mathematical-programming approach was developed and a convexification technique was proposed. Several case studies are solved to illustrate the ease, rigor, and applicability of the developed targeting technique.

The following recommendations are proposed for future work:

- Development of an algebraic technique for recycle problems with multiple fresh sources and multiple process sources
- Development of a non-iterative approach for multi-component and multi-property problems.

- Development of algebraic design rules to determine optimum extent of intercepting process sources
- Extension of developed techniques to problems with data uncertainty and to systems with dynamic performance.
- Extension of developed techniques to batch systems.

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